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POLYTECHNIQUE MONTRÉAL

affiliée à l'Université de Montréal

**Caractérisation d'une surface structurée non conductrice pour le support de
modes de surface térahertz**

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Mémoire présenté en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*

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présenté par **Mathieu POULIN**

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DÉDICACE

À mes parents ainsi qu'à ma bien-aimée Claudia

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RÉSUMÉ

Les ondes de surface se propageant le long d'une interface entre deux matériaux ont révolutionné divers domaines d'application pour leurs faibles tailles modales ainsi que leurs conditions de résonances. Particulièrement, ces modes excités aux interfaces entre un diélectrique et un métal, soit les plasmons polaritons de surface, sont exploités dans les domaines œuvrant dans les plages spectrales de l'infrarouge et du visible, telles que l'imagerie à super-résolutions, la détection ainsi que la conception de circuits électroniques de petite taille. Or, depuis ces dernières années, un effort considérable est appliqué dans la recherche ainsi que le développement d'applications exploitant la gamme spectrale des térahertz (0,1 THz – 10 THz), et ce, à l'aide du développement récent des méthodes de générations et de détections d'impulsions térahertz. En effet, cette plage peu exploitée présente un grand potentiel dans le domaine de la détection biochimique, la surveillance-qualité ainsi que la communication sans-fil à haut débit. En revanche, la génération d'ondes de surface dans la gamme spectrale des térahertz est problématique puisque les matériaux conducteurs possèdent des propriétés inadaptées pour le confinement du mode électromagnétique, où une forte délocalisation de l'énergie dans l'espace est observée. Ainsi, la recherche d'interfaces pour l'excitation des modes de surface confinés pour la gamme spectrale des térahertz est en ébullition. Ce mémoire a donc pour objectif de déterminer une telle interface capable de supporter des modes de surface pour cette plage fréquentielle ainsi que de caractériser les propriétés de ces derniers.

Pour trouver la solution, une revue critique de la littérature est effectuée afin d'évaluer des alternatives ainsi que les méthodes déjà explorées par la communauté scientifique. Suivant cette revue, il est évident que le choix d'utiliser un métamatériau (matériau possédant des structures périodiques de tailles plus petites que la longueur d'onde d'opération) pour le support de modes de surface est nécessaire puisque ce dernier offre un contrôle sur la valeur de la permittivité effective du matériau ainsi que permet le confinement de l'énergie dans ces structures. Dans le cadre de ce travail, une structure présentant des rainures périodiques de petite taille a été choisie comme métamatériau pour le support de modes de surface. De plus, puisque les métaux sont très absorbants dans le spectre des térahertz, l'hypothèse qu'un métamatériau non conducteur pourrait supporter des modes de surface localisés près de l'interface est émise. Pour vérifier cette hypothèse, une dérivation rigoureuse des équations de Maxwell est effectuée afin de retrouver une relation de

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Finalement, la caractérisation de ce métamatériau non conducteur propose le support d'un nouveau type de modes de surface encore jamais abordés dans la littérature. Ce dernier se distingue des quasi-ondes plasmoniques de surface, qui sont des modes de surface excités à l'interface entre un diélectrique et un métamatériau métallique utilisés pour les applications actuelles dans les gammes spectrales des térahertz, de l'infrarouge et du visible. Or, les modes de surface supportés par le métamatériau non conducteur se caractérisent par une forte localisation de l'énergie près de la surface et dans les rainures ainsi que par leurs propriétés flexibles qui sont fonctions des paramètres géométriques et optiques du métamatériau. Ce type de matériaux structurés non conducteurs pourrait remplacer les métamatériaux métalliques afin d'augmenter la performance des applications œuvrant dans la gamme spectrale des térahertz, telles que les détecteurs biochimiques, mais aussi de permettre l'imagerie térahertz ainsi que d'offrir un support compact pour le transport de l'information dans cette gamme spectrale, par exemple lors de la conception de systèmes de communication sans-fils.

ABSTRACT

The surface waves, which can propagate at the interface between two materials, have revolutionized multiple domains because of their small modal sizes and their resonance conditions. In particular, these surface modes excited at the interface between a dielectric and a conductor, called surface plasmon polaritons, are mainly used in applications working in infrared and visible spectral ranges, such as super-resolution imaging, sensing, and conception of compact electronic circuits. Since the last few years, important efforts have been applied in the search and development of new applications using the terahertz spectral range. Indeed, this frequency range shows enormous potentials in the growth of applications based on biochemical sensing, industrial imaging and security, and high-speed wireless communication. However, one can show that the generation of surface wave at the interface between a dielectric and a conductor is complicated in this spectral range as these modes tend to be highly delocalized (large modal size). So, to be able to exploit the surface wave in these previous applications, new interfaces able to support highly confined surface modes are needed. The goal of this thesis is thus to find an interface able to support such surface modes for the terahertz spectral range and to characterize the properties of the supported modes.

To find this interface, a critical review is first performed in order to evaluate possible solutions and to understand the initial works done by the scientific community. Then, based on the review, the use of metamaterial (material or surface with periodic structures with dimensions smaller than the operational wavelength) for the support of confined surface mode is selected as they offer great control on the effective permittivity of the material and allow the confinement of the energy inside the structure. In this work, a surface with periodic thin grooves is chosen as the metamaterial. Moreover, because conductors are highly lossy in the terahertz spectral range, the hypothesis that the corrugated surface made of non-conducting material could be able to support highly confined surface modes is discussed. To validate this hypothesis, a rigorous derivation of the Maxwell equations is performed to retrieve the dispersion relation and to evaluate the properties of such supported surface modes. Also, numerical simulations with the software COMSOL are performed to find the electromagnetic solutions supported by the metamaterial made of non-conducting material. The analytical and numerical solutions are compared to validate the hypothesis.

concerning the support and propagation of highly confined surface modes on the metamaterial. The limitations of the analytical formulations are also discussed.

Finally, the characterization of this metamaterial made of non conducting material reveal the support of a new kind of surface modes. It is physically different from the well-known spoof surface plasmon polariton, which is a surface mode propagating at the interface between a dielectric and a metamaterial made of conductors that can be excited at various spectral ranges, such as terahertz, infrared and visible. The new kind of surface modes are characterized by their highly confined energy near the interface and in the grooves of the structure. Moreover, their properties are flexible and depend on the geometrical and optical parameters of the metamaterial. This non conducting corrugated material could replace the metallic ones in order to improve the performance of various applications working in the terahertz spectral range, such as biochemical sensing, terahertz imaging and wireless communication devices.

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LISTE DES SIGLES ET ABRÉVIATIONS

ADN	Acide désoxyribonucléique
ARN	Acide ribonucléique
CGS	Système centimètre-gramme-seconde
CW	Onde entretenue
E&M	Électromagnétique
IBC	Condition aux limites d'impédance
IR	Infrarouge
PEC	Conducteur électrique parfait
PML	Couche absorbante parfaitement adaptée
RIU	Unité d'indice de réfraction
SPP	Plasmons polaritons de surface
SPR	Résonance plasmonique de surface
THz	Téraherz
THz-TDS	Spectroscopie dans le domaine du temps pour la gamme spectrale des térahertz
TM	Magnétique transverse

CHAPITRE 1 INTRODUCTION

Les guides d'ondes électromagnétiques correspondent à des structures permettant de confiner ainsi que de diriger des modes électromagnétiques, où les solutions sont obtenues à l'aide des équations de Maxwell. En particulier, il est possible de simplement confiner un mode à l'interface entre deux matériaux. Ces ondes de surface se caractérisent par la localisation de l'énergie à l'interface ainsi que par leur capacité à se propager aisément le long de la limitation entre les deux milieux. Les phénomènes physiques impliqués dans l'excitation de tels modes, quant à eux, dépendent des types de matériaux employés ainsi que de la fréquence d'opération. Notamment, dans le spectre du visible, une onde de surface peut être excitée et guidée le long de l'interface entre un diélectrique et un matériau conducteur, où un couplage entre une onde transverse magnétique à la surface (polariton) et l'oscillation électronique dans le conducteur (plasmon) est obtenu. Ces derniers, portant le nom de plasmons polaritons de surface, ont été grandement étudiés ainsi qu'exploités dans diverses domaines œuvrant dans les gammes spectrales de l'infrarouge ainsi que du visible [1]. Par exemple, la faible taille modale de ces ondes de surface (pouvant atteindre des dimensions plus petites que la longueur d'onde d'opération) offre la possibilité de réduire l'ordre de grandeur des composants optoélectroniques [2-5] ainsi que de concevoir des systèmes d'imagerie à super-résolution (dépassement de la limite de diffraction) [6-9]. Les conditions de résonance de ces modes de surface, quant à eux, sont aussi exploitées dans les domaines de détections sans contacts pour leur grande sensibilité à la variation de la permittivité des milieux [10, 11].

Récemment, le développement d'outils et de méthodologies permettant l'excitation et la détection d'ondes électromagnétiques dans la gamme spectrale des térahertz (0,1 THz à 10 THz) a grandement accéléré le développement technologique dans plusieurs domaines pouvant bénéficier de cette plage fréquentielle [12, 13]. Tout d'abord, les domaines industriels de l'imagerie et de l'inspection non destructive peuvent bénéficier de cette gamme spectrale pour leur pénétration importante dans une vaste gamme de diélectriques ainsi que leur grande résolution spatiale (comparativement aux micro-ondes) [14-16]. Aussi, les molécules d'eau présentent une absorption élevée des sources d'excitation térahertz [17, 18] et possèdent des fréquences de résonances intramoléculaires de l'ordre des térahertz en phase gazeuse [19], permettant alors une surveillance de haute sensibilité dans les industries agroalimentaires, par exemple par la détection de

moisissures, de bactéries ou encore de contaminations dans l'eau [20, 21]. En fait, beaucoup de molécules présentent des fréquences de résonances dans cette plage fréquentielle, motivant alors le développement des méthodes d'imageries et de détections térahertz dans le domaine biomédical [22-24]. Enfin, avec pour objectif d'augmenter la capacité d'échange d'information dans le domaine de la communication, l'augmentation des fréquences employées correspond à une option intéressante pour le transport de l'information sans-fil à haut débit [25-27] ainsi que dans les systèmes optoélectroniques et les circuits intégrés [28].

Or, tous ces domaines d'expertises peuvent aussi bénéficier des ondes de surface pour la réduction de la taille des systèmes de transport d'ondes électromagnétiques [29, 30], l'imagerie térahertz à super-résolution [31] ainsi que l'exploitation des conditions de résonances pour la détection biologique [32]. Cependant, les plasmons polaritons de surface ne peuvent pas être exploités dans cette gamme spectrale prometteuse, où l'énergie est largement délocalisée aux interfaces entre les diélectriques et les matériaux conducteurs découlant de la faible pénétration des champs dans les métaux. Une recherche intensive est donc nécessaire pour la conception de nouveaux matériaux pour le support d'ondes de surface térahertz ayant des propriétés similaires à ceux des plasmons polaritons de surface que l'on retrouve dans les plages spectrales de l'infrarouge et du visible.

Ainsi, l'objectif de ce mémoire est de déterminer et caractériser une interface capable de supporter des ondes de surface dans la gamme spectrale des térahertz. De plus, afin de permettre la conception de nouvelles applications térahertz, ces dernières doivent présenter des caractéristiques similaires à ceux des plasmons polaritons de surface pouvant être excités dans le visible, soit la capacité de se propager le long d'une interface ainsi que de posséder de petites tailles modales (localisation importante de l'énergie à l'interface). Suivant une recherche intensive dans la littérature afin de regrouper les approches déjà explorées par la communauté scientifique ainsi que d'évaluer les approches possibles, un métamatériau non conducteur est proposé pour le support de modes de surfaces térahertz. Ce dernier correspond à un matériau diélectrique possédant des gravures périodiques de tailles plus petites que la longueur d'onde d'opération. Un développement rigoureux des équations de Maxwell ainsi que des simulations numériques de cette structure révèlent le support de modes de résonances ayant des propriétés similaires aux ondes de surface analogues. Ainsi, ce métamatériau non conducteur capable de supporter des modes de surface dans la plage spectrale des térahertz correspond à une toute nouvelle approche innovatrice présentant un grand potentiel dans le développement de divers domaines œuvrant dans les térahertz.

CHAPITRE 2 REVUE CRITIQUE DE LA LITTÉRATURE

Ce chapitre correspond à un condensé de la revue critique de la littérature entourant les ondes de surface, les métamatériaux ainsi que les applications potentielles pouvant bénéficier de ces modes de surface dans la gamme spectrale des térahertz. Plus particulièrement, la relation de dispersion ainsi que les conditions d'existence de ces derniers sont obtenues à l'aide des équations de Maxwell, une liste de métamatériaux utilisés pour le support de modes de surface est présentée et plusieurs domaines pouvant bénéficier de ces ondes de surface sont discutées. Une revue de littérature additionnelle est aussi présentée sous forme d'un article scientifique dans le Chapitre 4, basé sur la recherche d'une solution pour l'excitation de modes de surface localisés.

2.1 Classification des ondes de surface

Les ondes de surface correspondent à une solution des équations de Maxwell pour une interface entre deux matériaux ayant des constantes de permittivité différentes. Cette solution est généralement caractérisée par une forte localisation de l'énergie à l'interface, associée à une constante de propagation complexe orientée parallèlement aux surfaces. De plus, la distribution transverse du champ se traduit par deux ondes évanescentes, dont l'amplitude décroît exponentiellement de l'interface. La Figure 2.1 illustre le problème à résoudre ainsi que la distribution de l'énergie d'une onde de surface se propageant le long d'une interface entre deux matériaux de permittivités différentes.

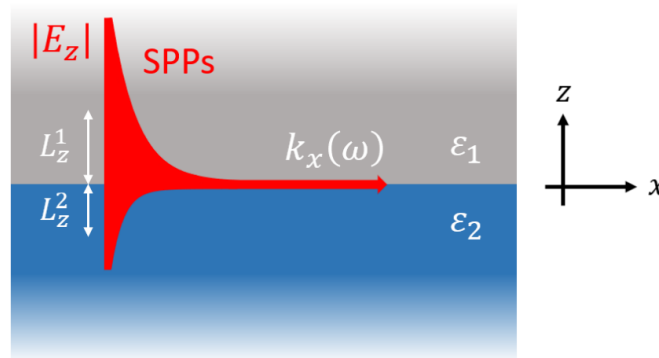


Figure 2.1 Illustration d'un SPPs (plasmons polaritons de surface) se propageant le long d'une interface entre deux matériaux de constantes de permittivité ϵ_1 et ϵ_2 . La norme de la composante en z du champ électrique des ondes évanescentes transversales est illustrée en rouge.

Une relation de dispersion peut aisément être retrouvée en résolvant les équations de Maxwell (selon le système d'unités CGS) [33] :

$$\begin{cases} \nabla \times \mathbf{E}(\mathbf{r}, t) + \frac{\mu(\mathbf{r})}{c} \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t} = 0 \\ \nabla \times \mathbf{H}(\mathbf{r}, t) - \frac{\varepsilon(\mathbf{r})}{c} \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} = 0 \end{cases} \quad (2.1)$$

Pour une onde TM (transverse magnétique) se propageant dans le diélectrique dans le plan xz, le champ électrique ainsi que le champ magnétique correspondent à :

$$\begin{cases} \mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{i\mathbf{k} \cdot \mathbf{r} - i\omega t} \\ \mathbf{H}(\mathbf{r}, t) = \mathbf{H}_0 e^{i\mathbf{k} \cdot \mathbf{r} - i\omega t} \end{cases} \quad (2.2)$$

où $\mathbf{k} = (k_x, 0, k_z)$ est le vecteur d'onde et $\mathbf{E}_0 = (E_x^0, 0, E_z^0)$ ainsi que $\mathbf{H}_0 = (0, H_y^0, 0)$ sont des constantes liées aux amplitudes des champs. En combinant les Équations 2.1 et 2.2, des relations entre les amplitudes $\mathbf{E}_0$ et $\mathbf{H}_0$, la constante de permittivité ε et le vecteur d'onde $\mathbf{k}$ sont obtenues :

$$\begin{cases} \nabla \times \mathbf{E}(\mathbf{r}, t) = ik_0 \mathbf{H}(\mathbf{r}, t) & \Rightarrow \mathbf{H}_0 = \frac{\mathbf{k} \times \mathbf{E}_0}{k_0} \\ \nabla \times \mathbf{H}(\mathbf{r}, t) = -ik_0 \varepsilon \mathbf{E}(\mathbf{r}, t) & \Rightarrow \mathbf{E}_0 = \frac{\mathbf{H}_0 \times \mathbf{k}}{\varepsilon k_0} \end{cases} \quad (2.3)$$

avec $k_0 = \omega/c$. Ainsi, une relation de dispersion s'obtient en résolvant le système d'Équations 2.3 :

$$(k_x)^2 = \varepsilon_{1,2} (k_0)^2 - (k_z^{1,2})^2 \quad (2.4)$$

où k_z^1 et k_z^2 correspondent aux composantes perpendiculaires des vecteurs d'onde se propageant respectivement dans les deux milieux de permittivités différentes ε_1 et ε_2 , $k_x = n_{eff} k_0$ correspond à la constante de propagation complexe de l'onde et n_{eff} est l'indice de réfraction effective du mode. De plus, la condition de continuité du champ parallèle à l'interface formée par les deux matériaux doit être respectée, menant à une condition supplémentaire :

$$\varepsilon_2 k_z^1 = \varepsilon_1 k_z^2 \quad (2.5)$$

Enfin, en combinant l'ensemble des conditions (Équations 2.4 et 2.5), on retrouve la relation de dispersion d'une onde de surface :

$$k_x = \frac{\omega}{c} \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}} \quad (2.6)$$

Aussi, afin d'obtenir des ondes évanescentes ainsi qu'une localisation de l'énergie à l'interface, l'amplitude des champs doit décroître dans les directions opposées à la surface. Ainsi, en considérant une interface à $z = 0$ telle qu'illustrée à la Figure 2.1, une autre condition doit être respectée afin d'obtenir une onde de surface :

$$\begin{cases} \text{Im}(k_z^1) < 0, & z > 0 \\ \text{Im}(k_z^2) > 0, & z < 0 \end{cases} \quad (2.7)$$

Finalement, afin de caractériser les propriétés de ces modes de surfaces, il est usuel de définir les tailles modales comme étant la distance à laquelle l'amplitude du champ décroît d'un facteur e . Puisque les champs sont harmoniques, ces dernières peuvent être définies comme suit :

$$L_z^{1,2} = 1/|\text{imag}(k_z^{1,2})| \quad (2.8)$$

Ici, il est important de noter que la présence d'ondes évanescentes demande des vecteurs d'ondes complexes (Équation 2.7). En combinant ce critère avec les Équations 2.4 et 2.6, on obtient une relation importante concernant la possibilité de supporter des ondes de surface entre deux matériaux :

$$\left| \text{imag} \left(\sqrt{\varepsilon_1} \sqrt{1 - \frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2}} \right) \right| > 0; \quad \left| \text{imag} \left(\sqrt{\varepsilon_2} \sqrt{1 - \frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2}} \right) \right| > 0 \quad (2.9)$$

Cette condition suggère, par exemple, qu'une onde de surface ne peut pas être excitée à l'interface entre deux matériaux ayant des constantes de permittivité purement réelles et positives. En revanche, l'Équation 2.9 est valide lorsque les deux matériaux possèdent des constantes de permittivité de signes opposés, ce qui est le cas pour la plupart des interfaces entre un diélectrique et un matériau conducteur dans les gammes spectrales de l'infrarouge et du visible. Physiquement, cette solution correspond à un couplage entre une onde E&M (électromagnétique) située à la surface et une oscillation électronique dans le métal. Ainsi, ce type d'onde de surface est communément appelé plasmons polaritons de surface [1]. Il est grandement exploité pour sa faible taille modale (pouvant être inférieure à celle de la longueur d'onde d'opération) dans diverses domaines, tels que l'imagerie à super-résolution [6], la détection [34-36] ainsi que la communication optoélectronique [3, 37, 38]. Il existe aussi des types additionnels d'ondes de surface pouvant se classifier en fonction des types de matériaux. Par exemple, une solution peut être obtenue à l'interface entre un diélectrique et un matériau polaire telle qu'un cristal, où un couplage entre une onde E&M et une vibration collective des atomes (phonon) est obtenu [39].

Cette onde de surface est alors référée dans la littérature comme des phonons polaritons de surface [40]. De plus, il est possible de localiser l'énergie à l'interface entre deux matériaux ayant des constantes de permittivité positives, à la condition qu'au moins l'un des deux soit absorbant ($|\text{imag}(\varepsilon)| > |\text{real}(\varepsilon)|$) afin de satisfaire à la condition 2.9. Dans ce cas-ci, ce mode de surface est possible à une condition physique particulière associée à l'angle entre les vecteurs d'ondes à l'interface permettant d'obtenir un coefficient de réflexion nulle. Cette valeur, appelée l'angle de Brewster, permet l'excitation d'une onde de surface communément nommé l'onde de Zenneck [41].

Finalement, il est à noter que la fréquence d'opération joue aussi un rôle important dans la classification des ondes de surface puisque la permittivité des matériaux est généralement dépendante de la fréquence. Par exemple, pour les métaux, la permittivité est décrite par le modèle de Drude, indiquant une dépendance à la fréquence d'opération ω ainsi qu'à la fréquence plasma ω_p du conducteur [42]. Ainsi, bien que les plasmons polaritons de surface soient bien définis dans le spectre du visible, l'énergie de ces derniers est largement délocalisée à la surface de l'interface lorsque la fréquence d'opération est de l'ordre des térahertz. Ce phénomène découle de la faible distance de pénétration du champ dans les matériaux conducteurs.

Une revue détaillée de ces différents types d'ondes de surface ainsi que de leurs propriétés dans la gamme spectrale des térahertz est présentée dans le Chapitre 4. Suivant cette revue, il en découle que les interfaces composées de matériaux homogènes, telles que les matériaux conducteurs, les matériaux polaires ainsi que les diélectriques absorbants ne peuvent pas supporter des ondes de surface présentant une forte localisation de l'énergie. Pour résoudre ce problème, il est alors nécessaire d'étudier les métamatériaux offrant un contrôle sur la permittivité effective du matériau.

2.2 Support de modes de surface à l'aide de métamatériaux pour les applications térahertz

Les métamatériaux correspondent à des matériaux composites possédant des structures de tailles plus petites que la longueur d'onde d'opération, permettant d'offrir des propriétés optiques uniques ne pouvant être retrouvées dans un matériau homogène naturel [43]. Du point de vue macroscopique, ce mélange de plusieurs matériaux de permittivités différentes s'apparente généralement à un milieu homogène ayant une permittivité effective ε_{eff} [44]. Ces combinaisons,

correspondant à des inclusions de nanoparticules dans un matériau hôte, ou encore d'un matériau usiné ayant des gravures structurées de petite taille, offre la possibilité de concevoir des milieux de permittivités effectives personnalisées. Or, puisque les métaux présentent des constantes de permittivités inadaptées pour le support d'onde de surface dans la plage fréquentielle des térahertz, l'utilisation de métamatériaux correspond à une solution viable pour la localisation de mode de surfaces [45].

Puisque les métamatériaux correspondent essentiellement à un matériau homogène du point de vue macroscopique, l'évaluation de la relation de dispersion d'une onde de surface (Équation 2.4) peut être appliquée, où la constante de permittivité du matériau fonctionnel est effective et dépendante de la composition ainsi que des paramètres géométriques la structure [46]. Cependant, bien que les propriétés des modes supportées soient similaires à ceux des ondes de surface se propageant le long d'une interface entre deux matériaux homogènes, il est à noter que la distribution des champs électriques et magnétiques est différente par l'aspect microscopique hétérogène du métamatériau. Ainsi, les solutions des équations de Maxwell correspondant à une localisation de l'énergie à l'interface entre un matériau homogène et un métamatériau sont plutôt classifiées comme étant des modes de surface. De plus, par leurs propriétés similaires à ceux des ondes de surface (tels que leurs tailles modales et leur distance de propagation), ces solutions sont aussi décrites comme des quasi-ondes de surface. Par exemple, dans la littérature, les modes de surface excités à l'interface entre un diélectrique et une surface métallique structurée sont souvent référés comme des quasi-ondes plasmoniques de surface [47].

Il existe plusieurs types de métamatériaux, chacun apportant leurs effets sur la relation de dispersion des modes de surfaces. Dans un premier temps, une première classe de métamatériaux correspond aux surfaces structurées à l'aide de rainures ou de trous périodiques de tailles plus petites que la longueur d'onde d'opération [48]. En général, ces cavités peuvent supporter des modes de résonances où l'énergie est majoritairement concentrée, permettant alors de réduire la délocalisation de l'énergie dans le deuxième milieu [49-51]. De plus, les rainures peuvent prendre plusieurs formes conçues pour maximiser la localisation de l'énergie dans les cavités, telles que des rainures rectangulaires [52], trapézoïdes [53], courbées [54] ainsi qu'en formes de « T » [55] et de « V » [56]. Des matériaux hôtes alternatifs, tels que les semiconducteurs, peuvent aussi être exploités pour le support de modes de surface [57, 58]. Ce type de matériaux offre un contrôle additionnel sur la relation de dispersion des modes grâce à leur concentration flexible de charges

[59, 60]. Ensuite, un deuxième type de métamatériaux intéressants pour le support de modes de surfaces correspond aux rubans structurés. Similairement aux surfaces présentant des gravures de petites dimensions, ces rubans métalliques possèdent des structures capables de supporter des modes de résonances ainsi que de confiner l'énergie [61, 62]. De plus, leurs flexibilités ainsi que leur capacité à guider des modes de surface sur de longues distances font d'eux d'excellents candidats dans la conception de guides d'ondes, et ce même dans la plage spectrale des térahertz [63]. Enfin, tout comme les surfaces structurées présentées plus tôt, les bandes peuvent prendre des structures de diverses formes, telles que des ouvertures rectangulaires [64], trapézoïdes [65], sphériques [66] ainsi qu'en formes de « T » [67]. Un dernier exemple de types de métamatériaux est le fil métallique structuré, où les structures de tailles plus petites que la longueur d'opération permettent le support de modes radiaux résonants. Similairement aux autres métamatériaux présentés, le champ E&M possède une distribution localisée autour du support et présente des propriétés similaires aux ondes de surface guidées [68]. Ces guides d'ondes peuvent prendre diverses formes, telles qu'une structure hélicoïdale [69], un fil cylindrique avec insertion d'anneaux creux pour localiser l'énergie [70], ou encore d'un guide d'ondes coaxial [71]. Ce type de métamatériaux est adapté pour le guidage de modes ainsi que la conception de sondes.

Il est à noter que les métamatériaux précédemment présentés sont majoritairement composés de métaux. L'un des avantages de ce choix de matériaux est la possibilité d'obtenir, avec précision, des structures périodiques de petite taille de l'ordre des micromètres à l'aide de méthodes de microfabrications, telles que la lithographie pour la définition de la structure sur une photorésine [72], le dépôt de couches minces métalliques par évaporation par faisceau d'électrons [73] ainsi que la gravure par ions [74]. Ces techniques combinées offrent la possibilité de concevoir des métamatériaux métalliques possédant des structures de taille plus petite que la longueur d'onde d'opération pour les domaines œuvrant dans les gammes spectrales d'intérêt.

2.3 Domaines d'application des ondes de surface dans la gamme spectrale des térahertz

La faible taille modale et les conditions de résonances des modes de surfaces peuvent être exploitées dans divers domaines œuvrant dans la gamme spectrale des térahertz, par exemple la détection [75, 76]. Pour commencer, la propagation d'une onde de surface le long d'une interface entre un matériau fonctionnel et une substance à analyser permet la détection non évasive de la

variation des propriétés de cette dernière [77]. En effet, puisque l'indice de réfraction effectif du mode n_{eff}^{SW} est fonction de l'indice de réfraction complexe de la matière à l'étude n_a , il existe une relation entre les pertes de propagation, le déphasage du mode de surface ainsi que l'indice de réfraction d'intérêt (ces types de détecteurs sont développés dans le Chapitre 4.4). Similairement, la variation de l'indice de réfraction peut aussi être détectée à l'aide des conditions d'excitation et de résonances de modes de surface [78]. En fait, pour obtenir un couplage entre une source d'excitation et un mode de surface, une correspondance entre les deux vecteurs de propagation d'onde est nécessaire. De plus, la relation de dispersion des modes de surface est dépendante de la fréquence d'opération, correspondant à une condition complémentaire pour l'excitation du mode. Dans la littérature, ce couplage sélectif est généralement associé à une résonance, d'où l'appellation de résonance plasmonique de surface [79]. Ce type de détection peut prendre plusieurs formes. La première repose sur le couplage entre un mode E&M se propageant dans un guide d'onde et une onde de surface à l'interface entre l'une des parois du guide d'onde et la substance à analyser [80]. Ici, le mode guidé est uniquement en fonction de la fréquence d'opération. Pour effectuer la détection, un spectre d'absorption doit donc être obtenu afin d'identifier la fréquence résonante avec le mode de surface. Une relation entre la fréquence de résonance et l'indice de réfraction du milieu d'intérêt est ainsi obtenue. La deuxième repose sur l'utilisation d'une source d'excitation incidente. Ce dernier a pour avantage supplémentaire de pouvoir exciter une onde de surface selon son angle d'incidence avec l'interface supportant le mode de résonance. Ainsi, la détection de la variation peut s'effectuer autant selon la fréquence de résonance [81] que selon l'angle d'incidence [82]. Or, puisque les ondes de surface excitées dans la gamme térahertz sont généralement lentes ($n_{eff} > n_a$), le couplage doit s'effectuer dans un milieu d'indice de réfraction supérieur. Pour satisfaire à cette demande, l'utilisation d'un prisme de couplage est employé [83]. Ce type de couplage permet aussi de choisir le matériau fonctionnel destiné à supporter le mode de surface. Ainsi, les métamatériaux peuvent aisément être employés avec ce type de détecteur [84].

Par la suite, lorsque la taille modale du mode de surface est inférieure à la longueur d'onde d'opération ($L_z < \lambda$), il est possible de sonder une surface avec une résolution supérieure à celle théoriquement dictée par la limite de diffraction optique de la source [6]. Dans un tel cas, l'onde évanescente du mode de surface est exploitée pour interagir avec la surface à courte portée. Cette interaction de taille plus petite que la longueur d'onde d'opération permet alors l'imagerie à super-résolution. Cette technique se caractérise par la génération d'un mode de surface à courte portée de

la surface d'intérêt, puis de la mesure de l'interaction. Cette dernière correspond généralement à la mesure du spectre de réflexion ou de transmission de champ à l'aide d'un détecteur éloigné, permettant alors l'identification de la fréquence de résonance du mode. Or, l'excitation des modes peut s'effectuer de plusieurs façons, par exemple à l'aide d'une sonde structurée capable de supporter des modes de surface ainsi que de focaliser l'énergie en un point sur la surface [85]. La recherche de matériaux fonctionnels capables de supporter des modes de surfaces est donc critique pour le développement de ces applications œuvrant dans les térahertz. De plus, ces guides d'ondes compacts peuvent servir dans la miniaturisation des systèmes précédemment présentés, où les modes de surface dans la gamme spectrale des térahertz sont généralement délocalisés dans l'espace, ainsi que pour accompagner les systèmes de communications sans-fil à hautes fréquences [25-27].

CHAPITRE 3 DÉMARCHES ASSOCIÉES À LA RÉOLUTION DU PROBLÈME ET À LA CARACTÉRISATION DE LA SOLUTION

Dans les prochains chapitres qui suivent, les différents éléments concernant la problématique soulevée dans ce mémoire sont développés dans l'objectif de décrire, avec cohérence, le processus de recherche employé lors de la recherche de la solution. Pour commencer, une revue critique de la littérature entourant les matériaux disponibles pour le support d'ondes de surface dans la gamme spectrale térahertz a été rédigée et publiée dans le journal scientifique « MDPI Sensors ». Ce premier travail a pour but de justifier la recherche de matériaux pour le support d'ondes de surface pour la gamme spectrale d'intérêt, de présenter une revue de plusieurs types de matériaux potentiels, ainsi que d'évaluer théoriquement les propriétés des ondes de surface pour chaque type d'interface relevé. Ce premier ouvrage est d'une grande importance car elle révèle la pertinence de l'objectif de la recherche, tout en offrant des pistes de solutions concernant le type d'interface permettant de supporter des ondes de surface pour la gamme spectrale des térahertz.

Par la suite, basé sur l'ensemble des conclusions du premier ouvrage, un type de matériau a été retenu pour le support d'onde de surface, soit un matériau non conducteur possédant des structures de taille plus petite que celle de la longueur d'opération (métamatériau). Dans un premier temps, le choix d'utiliser un métamatériau se base sur sa flexibilité lors de sa conception, permettant d'avoir un contrôle sur les propriétés effectives du matériau, et donc sur les propriétés des modes de surface. En effet, tels qu'observés lors de la revue de littérature concernant les matériaux homogènes, les modes de surface classiques tels que les plasmons polaritons de surface et les phonons polaritons de surfaces possèdent des propriétés non adaptées pour les domaines œuvrant dans les térahertz. Le choix d'utiliser un métamatériau pour le support de modes de surface est donc nécessaire. Dans un deuxième temps, le choix d'utiliser des matériaux non conducteurs découle de deux observations. La première concerne le fait que la plupart des métamatériaux étudiés dans le domaine scientifique sont composés de métaux, et ce, même dans la plage spectrale des térahertz. Cette tendance s'explique par l'explosion de l'étude ainsi que du potentiel important entourant les quasi-ondes plasmoniques de surface, correspondant à des modes de surface ayant des propriétés analogues aux ondes de surface se propageant le long d'une interface entre un diélectrique et un métal. Ce mode supporté à la surface d'une métasurface a été grandement utile

pour le développement de diverses applications pour sa faible taille modale ainsi que ses conditions de résonances dans les spectres de l'infrarouge et du visible. Or, ses applications sont limitées dans les térahertz puisque la distribution de l'énergie des modes de surface est largement délocalisée dans l'espace, ce qui a fructifié l'idée d'opter pour un matériau non conducteur. La deuxième observation ayant justifié le choix d'étudier les modes de surface supportés par une surface structurée non conductrice repose sur les propriétés de ce dernier dans les térahertz. En effet, les métaux ont des valeurs de permittivités très grandes dans les térahertz. Ainsi, lors de la résolution analytique (ou numérique) du problème électromagnétique, il est usuel d'approximer les métaux par des conducteurs électriques parfaits ($|\epsilon_m| \rightarrow \infty$), permettant de grandement simplifier le problème ainsi que d'obtenir une relation de dispersion analytique [86]. Or, ces approximations analytiques proposent généralement des modes de surface lentes, signifiant que l'indice de réfraction effectif du mode est supérieur à celle du diélectrique entourant le métamatériau [87]. La dérivation d'une relation de dispersion sans effectuer cette dernière approximation est donc intéressante et pourrait servir à définir un nouveau type d'onde de surface. Dans un dernier temps, la conception d'une métasurface composée uniquement de diélectriques pour le support de modes de surface térahertz a été très peu étudiée dans la littérature. Or, ce dernier permettrait l'utilisation de matériaux alternatifs, tels que les céramiques, qui sont disponibles en abondance et présentant des pertes de propagations inférieures à celles des métaux dans la gamme spectrale des térahertz.

CHAPITRE 4 ARTICLE 1 : SURFACE WAVE ENHANCED SENSING IN THE TERAHERTZ SPECTRAL RANGE: MODALITIES, MATERIALS, AND PERSPECTIVES

L'objectif de recherche étant de trouver un support capable de supporter des ondes de surface dédiées pour diverses applications œuvrant dans la gamme spectrale des térahertz, une revue en littérature des avancées dans ce domaine est nécessaire. Or, afin d'évaluer les propriétés des différents types d'ondes de surface retenus de la littérature, ces dernières sont appliquées pour la conception théorique de détecteurs simplifiés. Ainsi, pour chaque combinaison d'interfaces pouvant supporter des modes de surface, une théorie basée sur la résolution des équations de Maxwell ainsi que les propriétés des modes en fonction de la fréquence d'opération et des matériaux employés sont présentées. Cette revue, publiée dans le journal scientifique « MDPI Sensors », a permis d'identifier une solution, soit la conception d'un métamatériau pour le support de modes de surface. De plus, suivant l'analyse des propriétés des métaux, des semiconducteurs ainsi que des matériaux polaires dans la gamme spectrale des térahertz, la considération d'utiliser des diélectriques pour la conception du métamatériau fût évoquée.

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4.2 Abstract

The terahertz spectral range (frequencies of 0.1–10 THz) has recently emerged as the next frontier in non-destructive imaging and sensing. Here, we review amplitude-based and phase-based sensing modalities in the context of the surface wave enhanced sensing in the terahertz frequency band. A variety of surface waves are considered including surface plasmon polaritons on metals, semiconductors, and zero gap materials, surface phonon polaritons on polaritonic materials, Zenneck waves on high-k dielectrics, as well as spoof surface plasmons and spoof Zenneck waves

on structured interfaces. Special attention is paid to the trade-off between surface wave localization and sensor sensitivity. Furthermore, a detailed theoretical analysis of the surface wave optical properties as well as the sensitivity of sensors based on such waves is supplemented with many examples related to naturally occurring and artificial materials. We believe our review can be of interest to scientists pursuing research in novel high-performance sensor designs operating at frequencies beyond the visible/IR band.

4.3 Introduction

The extreme spatial confinement of surface plasmon polaritons (SPPs) in the visible spectral range has led to a revolution in sensing [1]. Plasmonic waves propagate along the metal/dielectric interface, featuring a deeply sub-wavelength (100 nm–1 μ m) modal size [3, 11, 34], and optical properties that are highly sensitive to changes in the refractive index or geometrical structure of the analyte in the direct vicinity of the metal surface. These properties make surface plasmon polaritons ideal for high-sensitivity surface sensing applications and characterization of deeply sub-micron-sized objects (such as proteins, cell organelles, viruses, etc.) that have been immobilized or captured at the metal surface [88]. At the same time, due to extreme confinement of plasmons in the visible spectral range, they are not optimal for measuring bulk properties of a neighbouring analyte nor characterization of the larger super-1 μ m size objects (such as bacteria, dust particles, etc.).

Recently, the THz spectral range (frequencies of 0.1–10 THz, wavelengths of 3 mm–30 μ m) has emerged as the next frontier in non-destructive imaging and sensing. Key advantages when operating in the THz band are the ability to detect the complex electric field of THz waves (phase and amplitude), availability of both pulsed (sub-1 ps) and continuous wave (CW) THz systems, as well as ability of conducting dynamic measurements with sub-1 ms temporal resolution [13]. Additionally, relative transparency of dry dielectrics to THz radiation, strong absorption of THz waves by water and other polar solutions, as well as the non-ionizing nature of THz light enable many applications in non-destructive 2D imaging, 3D tomography, industrial sensing, bio-imaging/sensing, and security [78]. In the context of surface sensing, due to a relatively large size of THz waves, they can be used, in principle, for detection, characterization, and dynamic monitoring of changes in super-micron-sized objects (such as bacteria, cells, micro-organisms and some organelles, fine powders, aerosols, suspensions, condensates, etc.) conveniently localized on

a flat surface [89]. Unfortunately, generation of highly-confined surface modes using simple metals (ex. gold, silver) proved to be challenging in the THz spectral range. This is because, in the THz band, the dielectric constant of most simple metals is almost purely imaginary in contrast to the visible spectral range where it is almost purely real and negative. While excitation of surface waves at the metal surface in THz is still possible, such waves tend to significantly extend into the neighboring dielectric (100–1000 wavelengths) [42]. Such surface modes also tend to have low loss (defined by the dielectric material) and can be used in principle for bulk sensing applications.

The main goal of this paper is to go beyond surface plasmon polaritons at the interface with simple metals. In what follows we present a critical comparative analysis of alternative materials, different surface wave types, and sensor modalities that could be used to design surface wave enhanced sensors operating in the THz spectral range. We demonstrate that very different surface sensing modalities can be realized in the THz band that are characterized by different degrees of field localization in the vicinity of the material surface. Thus, true surface sensors with sub-wavelength probing depths can be realized using surface plasmon polaritons on semiconductors and zero-gap materials, surface phonon polaritons on polaritonic materials, as well as spoof plasmons and spoof Zenneck waves on structured materials with high absolute values of the dielectric constant. At the same time, bulk sensors that utilize surface waves with super-wavelength probing depths can be realized using surface plasmon polaritons on simple metals, as well as Zenneck waves on high-k dielectrics and polaritonic materials.

The paper is structured as follows: we first present a theoretical foundation for the amplitude and phase-based sensor detection modalities, and then develop expressions for the corresponding sensor sensitivities. We then present a brief theory of surface waves, their classification, and their optical properties such as modal size and modal propagation distance. Next, for each wave type we consider natural or artificial materials that can be used for its realization in the THz spectral range, as well as surface wave optical properties as related to such practical materials. Finally, we summarize our findings by classifying different wave types according to their potential in the surface or bulk sensing applications as well as projected sensitivity.

4.4 Amplitude and phase-based sensor modalities using surface waves

Here we consider a subset of sensors that use surface waves to detect and quantify changes in the refractive index of a neighboring analyte. The wave is assumed to propagate at the interface between a functional material (such as metal, semiconductor, etc.) and a simple dielectric (analyte) characterized by the refractive index n_d . The complex effective refractive index of a surface mode is defined as $n_{eff}(n_d)$ and both its real part (phase) and its imaginary parts (loss) are sensitive to the variation in the refractive index of a dielectric medium.

As complex dispersion relations for many surface waves are known analytically, then surface wave sensitivity to changes in the analyte refractive index can also be derived in the analytical form. This allows intimate understanding of the effects of material and design parameters on sensor performance. Importantly, the study of surface wave sensitivity should be supplemented with the analysis of surface wave extent into the analyte region, which determines the sensor probing depth and allows its characterization (somewhat ambiguously) as the “surface” or “bulk” sensor.

Alternatively, one can perform sensor characterization by studying surface wave sensitivity to changes in the thickness of a thin layer deposited at the interface. In fact, this modality is directly relatable to many practical implementations of the surface sensors. Theoretically, however, this arrangement is somewhat cumbersome to analyze as one must specify the refractive index the initial thickness of the deposited layer. The addition of these two free parameters makes analysis cumbersome and more graphical than analytical, which is the main reason why we chose a more theoretically elegant approach for the characterization of sensor sensitivity with respect to changes in the analyte refractive index complemented by the study of the surface wave probing depth.

4.4.1 Amplitude sensing modality

Amplitude sensing modality offers the simplest sensor implementation as it only requires monitoring of the sensor transmission amplitude. A simplified schematic of an amplitude-based sensor is presented in Figure 4.1. The amplitude sensing detection modality is mostly used to detect variations in the imaginary part of the analyte refractive index.

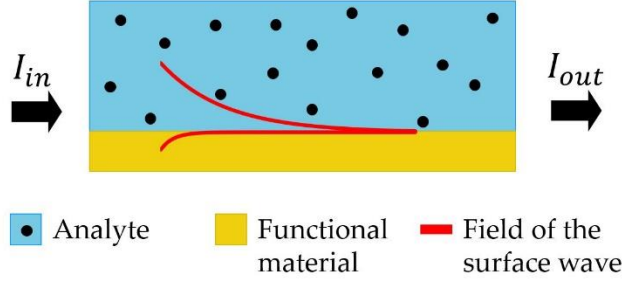


Figure 4.1 Schematic of an amplitude sensitive detection strategy. A light source is used to excite the surface mode at the interface between functional material and analyte. Variations in the transmitted amplitude is used to monitor changes in the analyte refractive index.

Within the amplitude-based modality, a small variation in the refractive index δn of the analyte can be quantified by measuring changes in the modal transmission loss $\alpha(n_d)$, which is, in turn, related to the imaginary part of the surface mode effective refractive index $n_{eff}^i(n_d)$ as:

$$n_{eff}(n_d) = n_{eff}^r(n_d) + in_{eff}^i(n_d) \quad (4.1)$$

$$\alpha(n_d) = k_0 n_{eff}^i(n_d) \quad ; \quad k_0 = \omega/c \quad (4.2)$$

Transmission losses can be obtained by monitoring intensity of the transmitted light I_{out} at the sensor output end as:

$$I_{out}(n_d + \delta n_d) = I_{in} e^{-2\alpha(n_d + \delta n_d)L} \quad (4.3)$$

where I_{in} is the light intensity at the sensor input end, and L is the sensor length. Thus, by comparing light intensities before $I_{out}(n_d)$ and after $I_{out}(n_d + \delta n_d)$ changes in the analyte refractive index took place, from Equation 4.3 we can write:

$$\frac{I_{out}(n_d + \delta n_d)}{I_{out}(n_d)} = \exp\left(-2 \frac{\partial \alpha(n_d)}{\partial n_d} L \cdot \delta n_d\right) = e^{-S^A \delta n_d} \quad (4.4)$$

where parameter S^A characterizes the amplitude sensitivity and is proportional to the sensor length. Recognizing that the maximal sensor length L_{max} is limited by the propagation loss of the surface mode:

$$L_{max} \sim \frac{1}{\alpha(n_d)} \quad (4.5)$$

We can estimate the maximal value of the amplitude sensitivity and relate it to the modal refractive index (using Equations 4.1 and 4.2) as:

$$S_{max}^A \left[\frac{1}{RIU} \right] = 2 \frac{\partial \alpha(n_d)}{\partial n_d} L_{max} = \frac{2}{n_{eff}^i(n_d)} \frac{\partial n_{eff}^i(n_d)}{\partial n_d} \quad (4.6)$$

Finally, Equation 4.4 also allows us to estimate sensor resolution. Particularly, defining $(\delta I/I)_{min}$ to be the smallest reliably detectable difference in the relative amplitude (which is typically smaller than 0.01), from Equation 4.4 it follows that the smallest detectable change in the analyte refractive index will be:

$$(\delta n_d)_A^A_{min} \sim \frac{(\delta I/I)_{min}}{S_{max}^A} \quad (4.7)$$

4.4.2 Phase sensing modality

Phase sensing modality, compared to amplitude-based strategy, offers a considerably more precise and better controlled technique for monitoring changes in the analyte refractive index. A simplified schematic of the phase-based sensor is presented in Figure 4.2. In such a sensor one frequently uses a Mach–Zehnder interferometer to convert a relative phase difference of light traveling along the reference and sensing pathways into an easily detectable amplitude variation. Phase sensing detection modality is, therefore, mostly used to detect variations in the real part of the analyte refractive index.

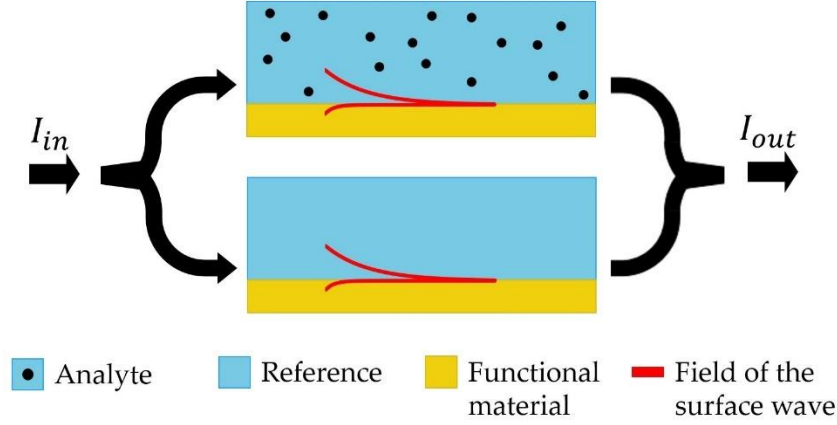


Figure 4.2 Schematic of a phase sensitive detection strategy. Coherent light is subdivided in two beams, one propagating through the reference and another through a sensor. The two beams are then recombined and resulting interference pattern is used to monitor variation in the analyte refractive index.

To introduce the phase sensitivity parameter, we have to analyze amplitude of the detected signal at the output of a Mach-Zehnder interferometer shown in Figure 4.2. Particularly, the electric fields after propagation along the length L in the reference and sensing branches of the interferometer are given by:

$$E(n_d, L) = E_{in} e^{ik_0 n_{eff}(n_d) L} \quad (4.8)$$

$$E(n_d + \delta n_d, L) = E_{in} e^{ik_0 n_{eff}(n_d + \delta n_d) L} \quad (4.9)$$

Assuming that the two branches show similar losses ($\alpha(n_d) \approx \alpha(n_d + \delta n_d)$), then the interference of light coming from the two branches will result in the following output intensity:

$$\begin{aligned} I_{out}(n_d + \delta n_d) &= |E(n_d) + E(n_d + \delta n_d)|^2 \\ &= 4E_{in}^2 \exp(-2\alpha(n_d)L) \cos\left(\frac{k_0 L}{2} \frac{\partial n_{eff}^r(n_d)}{\partial n_d} \delta n_d\right) = 4E_{in}^2 \exp(-2\alpha(n_d)L) \cos(S^P \delta n_d) \end{aligned} \quad (4.10)$$

Here, parameter S^P characterizes the phase sensitivity and is proportional to the sensor length. Recognizing that the maximal sensor length L_{max} is limited by the propagation loss of the surface mode $L_{max} \sim 1/\alpha(n_d)$, and using Equation 4.2, the maximal phase sensitivity can be estimated as:

$$S_{max}^P \left[\frac{rad}{RIU} \right] = \frac{k_0 L_{max}}{2} \frac{\partial n_{eff}^r(n_d)}{\partial n_d} = \frac{1}{2n_{eff}^i(n_d)} \frac{\partial n_{eff}^r(n_d)}{\partial n_d} \quad (4.11)$$

Finally, Equation 4.10 also allows us to estimate sensor resolution. Particularly, defining $\delta\varphi_{min}$ to be the smallest reliably detectable variation in the phase of an output signal (which is normally much smaller than π), from Equation 4.10 it follows that the smallest detectable change in the analyte refractive index will be:

$$(\delta n_d)_P^P_{min} \sim \frac{\delta\varphi_{min}}{S_{max}^P} \quad (4.12)$$

4.5 Theory of surface waves in the context of sensing applications

In what follows, we analyze the performance characteristics and application scenarios of the amplitude and phase sensing techniques described in the previous sections in the context of surface waves propagating at the interface between a functional material and an analyte (see Figures 4.1 and 4.2). Particularly, we aim at understanding the fundamental relations between the sensor sensitivity, the extent of the modal field of a surface wave into the analyte, and the maximal propagation length of a surface wave. Also, we consider a sensor to be a “surface sensor” if the modal field extent of a surface wave into the analyte (probing depth) is subwavelength or at most several wavelengths, while we consider a sensor to be a “bulk sensor” if the modal field extent of a surface wave into the analyte is many wavelengths. Remarkably, we find that in the case of low-loss analytes, and for many types of surface waves, sensor sensitivity correlates strongly with the modal probing depth. Thus, bulk sensors characterized by long probing depths tend to have higher sensitivities than the surface sensors characterized by subwavelength probing depths.

4.5.1 Dispersion relation of surface waves

Interaction between electromagnetic (E and M) waves and free charge carriers can yield surface plasmon polaritons (SPP) excitation at the metal or semiconductor/dielectric interfaces, while interaction of E and M waves with lattice vibrational modes lead to surface phonon polaritons at the polar media/dielectric interface. Moreover, well-confined surface-bound E and M states can be excited at the interface with a high-k dielectric having high material losses, which are known as a Zenneck surface waves. Finally, surface waves can be excited at the interface with a naturally-occurring or artificially-structured anisotropic media, in which case such waves are known as Dyakonov surface waves. Each one of these surface waves has its advantages and limitations and requires a particular set of material properties for their excitation. Moreover, due to variations of

the material properties with frequency, such surface waves can have completely different optical properties depending on the frequency range of operation. In this work we focus specifically on surface waves in the THz spectral range.

We first review the necessary conditions for the excitation of surface waves at the interface between two distinct materials, one of them being lossless dielectric with positive dielectric permittivity ϵ_d and another material with dielectric permittivity ϵ_m that can have either negative real part (metal, semiconductor, polar media just above the resonance) or positive real part (polar media just below the resonance, high-k dielectric). Figure 4.3 shows planar interface between two materials (OXY plane), and a TM-polarized electromagnetic (E and M) wave that has the only component of its magnetic field directed along the OY axis.

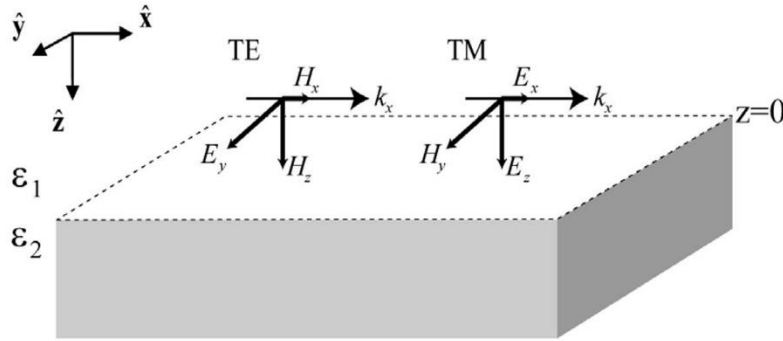


Figure 4.3 Schematic of an interface between two materials that guides a TM polarized surface wave.

On either side of the interface we assume a single TM polarized planewave of frequency ω and the corresponding E and M wavevectors $k_{d,m} = (k_x, 0, k_z^{d,m})$. The corresponding magnetic and electric fields on either side of the interface are given by:

$$\mathbf{H}_{d,m}(\mathbf{r}, t) = \hat{y} H_{d,m} e^{i k_{d,m} \mathbf{r} - i \omega t} \quad (4.13)$$

$$\mathbf{E}_{d,m}(\mathbf{r}, t) = \frac{\mathbf{H}_{d,m}(\mathbf{r}, t) \times \mathbf{k}_{d,m}}{\epsilon_{d,m} k_0} \quad (4.14)$$

where $k_0 = \omega/c = 2\pi/\lambda$, and the wavevectors satisfy the standard dispersion relations:

$$k_{d,m}^2 = \epsilon_{d,m} k_0^2 = k_x^2 + (k_z^{d,m})^2 \quad (4.15)$$

The E and M field components parallel to the interface must be continuous across the interface ($\hat{y}H_d(0, t) = \hat{y}H_m(0, t); \hat{x}E_d(0, t) = \hat{x}E_m(0, t)$), thus leading to the following equation for the $k_z^{(d,m)}$:

$$\frac{k_z^d}{\varepsilon_d} - \frac{k_z^m}{\varepsilon_m} = 0 \quad (4.16)$$

Using dispersion relations (Equation 4.15), as well as definition of the modal effective refractive index $k_x = n_{eff}k_0$, Equation 4.16 admits a simple analytical solution for the surface mode dispersion relation:

$$\varepsilon_{eff} = n_{eff}^2 = \frac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m} \quad ; \quad (k_z^{d,m})^2 = k_0^2 \frac{(\varepsilon_{d,m})^2}{\varepsilon_d + \varepsilon_m} \quad (4.17)$$

While Equation 4.17 is a solution of Equation 4.16, it does not necessarily describe a bound surface state as Equation 4.16 is just a condition of E and M field continuity across the interface. In order for Equation 4.17 to describe a surface state, one must require that the electromagnetic fields are decaying away from the interface (evanescent fields), which amounts to additional requirements:

$$\text{Im}(k_z^d) < 0 \quad ; \quad \text{Im}(k_z^m) > 0 \quad (4.18)$$

and define exponentially decaying fields in both media. Finally, for a surface-bound state we define its propagation length L_x as well as its extents into a dielectric L_d and a second material L_m as characteristic distances over which the E and M fields decay by the factor e :

$$L_x = \frac{1}{\text{Im}(k_x)} \quad ; \quad L_{d,m} = \frac{1}{\mp \text{Im}(k_z^{d,m})} \quad (4.19)$$

Now we detail several types of surface states propagating at the interface between a classic lossless dielectric with $\varepsilon_d > 0$ and a second material that can be either a metal, a polar material, a zero-gap material, or a lossy high-k dielectric. Particularly, in the case of simple Drude metals and semiconductors, their frequency-dependent dielectric constant is described as [42]:

$$\varepsilon_m(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \quad (4.20)$$

where ω_p is a plasma frequency and γ is a damping coefficient. Similarly, the dielectric constant of many polar materials near the resonance frequency ω_0 can be described using the Lorentz model:

$$\varepsilon_m(\omega) = 1 - \frac{\omega_p^2}{\omega^2 - \omega_0^2 + i\gamma\omega} \quad (4.21)$$

while lossy high-k dielectrics are characterized by $\varepsilon_m = \varepsilon'_m + i\varepsilon''_m$, where $\varepsilon'_m \gg 1$.

4.5.2 Lossless materials

We first consider the case of ideal (lossless) materials $\gamma = 0$ operating at frequencies where their dielectric constant is negative so that the two following conditions are satisfied $\varepsilon_m < 0$ and $\varepsilon_d + \varepsilon_m < 0$. In this case, the surface mode effective dielectric constant as given by Equation 4.17 is purely real and positive $\varepsilon_{eff} > \varepsilon_d$. For metals and polar materials, this limits the operation frequency to:

$$\text{Metals: } \omega < \frac{\omega_p}{\sqrt{1+\varepsilon_d}} \quad ; \quad \text{Polar materials: } \omega_0 < \omega < \sqrt{\omega_0^2 + \frac{\omega_p^2}{1+\varepsilon_d}} \quad (4.22)$$

At such frequencies, the OZ components of the two wavevectors are purely imaginary and their imaginary parts have the opposite signs:

$$k_z^{d,m} = \mp ik_0 \frac{|\varepsilon_{d,m}|}{\sqrt{|\varepsilon_m| - \varepsilon_d}} \quad (4.23)$$

thus defining a true surface state, which is called a surface plasmon polariton in case of metals and surface phonon polariton in case of polar materials. Electromagnetic fields of such a surface state decay exponentially fast away from the interface. The surface mode propagation length L_x is infinite as n_{eff} is purely real, while the surface mode extents into a dielectric L_d and a material L_m are given by Equation 4.24:

$$L_{d,m} = \frac{\lambda}{2\pi} \frac{\sqrt{|\varepsilon_m| - \varepsilon_d}}{|\varepsilon_{d,m}|} \quad (4.24)$$

Note that plasmon polariton or phonon polariton extents into the two media becomes deeply subwavelength $L_{d,m} \ll \lambda$ when $|\varepsilon_m| \sim \varepsilon_d$, which happens near the following frequencies:

$$\text{Metals: } \omega \sim \frac{\omega_p}{\sqrt{1+\varepsilon_d}} \quad ; \quad \text{Polar materials: } \omega \sim \sqrt{\omega_0^2 + \frac{\omega_p^2}{1+\varepsilon_d}} \quad (4.25)$$

In Figure 4.4 we present a typical lossless surface plasmon polariton dispersion relation as well as dependence of its penetration depths into a dielectric and metal as a function of frequency. The surface plasmon-polariton extent into metal is always deeply subwavelength $L_z^m \ll \lambda$, while its extent into the dielectric is generally comparable or even smaller than the wavelength of light $L_z^d < \lambda$ at higher frequencies.

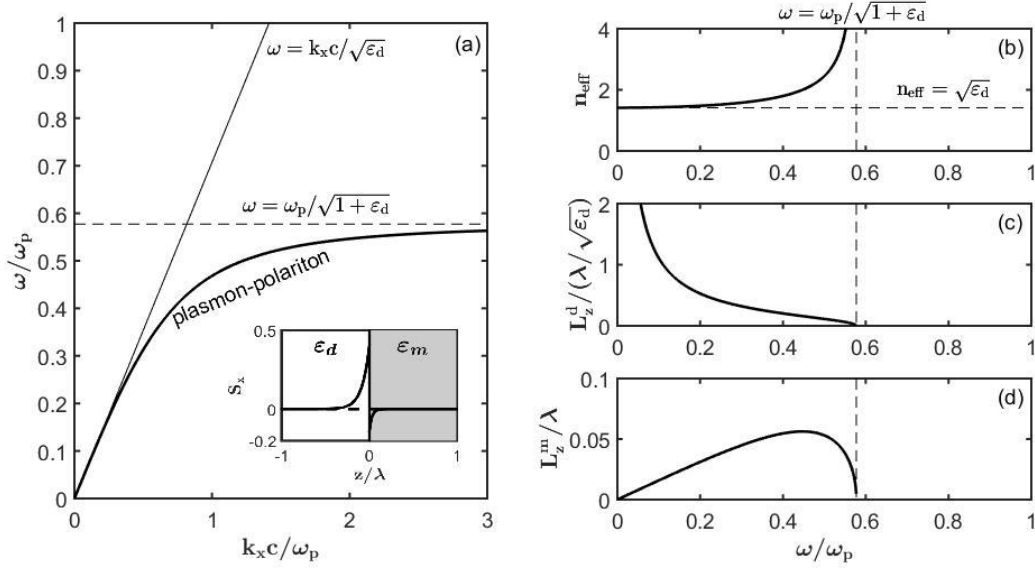


Figure 4.4 Dispersion relation and fundamental properties of a lossless surface plasmon polaritons ($n_d = 1.33$). (a) Band diagram of a surface plasmon. Insert: S_x energy flux of a plasmon at $\omega = 0.4\omega_p$. Optical properties of a plasmon: (b) Effective refractive index, (c) penetration depth into the dielectric, and (d) penetration depth into metal.

In Figure 4.5 we present similar results for a surface phonon polariton, and arrive to a similar conclusion that somewhat above the resonant frequency ω_0 , the surface phonon-polariton extent into a polar material is always deeply subwavelength $L_z^m \ll \lambda$, while its extent into the dielectric is generally comparable, or even smaller than the wavelength of light $L_z^d < \lambda$ at higher frequencies.

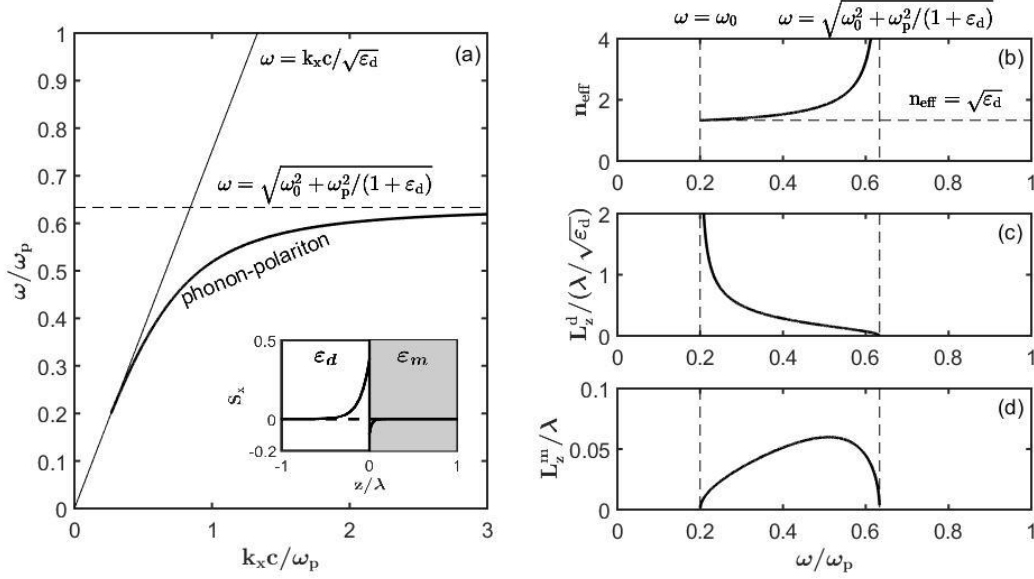


Figure 4.5 Dispersion relation and fundamental properties of a lossless surface phonon polariton ($n_d = 1.33$, $\omega_0 = 0.2\omega_p$). (a) Band diagram of a surface phonon polariton. Insert: S_x energy flux of a phonon polariton at $\omega = 0.4\omega_p$. Optical properties of a phonon polariton: (b) Effective refractive index, (c) penetration depth into the dielectric, and (d) penetration depth into the polar medium.

4.5.3 Lossy materials

When material losses are small:

$$\text{Metals: } \gamma \ll \frac{\omega_p}{\sqrt{1+\epsilon_d}} \quad ; \quad \text{Polar materials: } \gamma \ll \sqrt{\omega_0^2 + \frac{\omega_p^2}{1+\epsilon_d}} - \omega_0 \quad (4.26)$$

conclusions drawn in the case of lossless materials will still hold virtually unchanged, while corrections to the modal optical properties could be found using perturbative expansions with respect to the imaginary part of the dielectric constant. In some cases, however, material losses cannot be ignored as imaginary part of the material dielectric constant can be comparable or larger than its real part. This is notably the case of Drude metals at very low frequencies $\omega \ll \gamma$ operating in the THz and microwave spectral ranges. At such frequencies, the metal dielectric constant is essentially purely imaginary. Remarkably, even at very low frequencies a well-defined surface state with complex dispersion (Equation 4.17) still exists, as we will see in the following sections.

4.5.4 Lossy high-k dielectrics

A lossy surface-bound E and M state (also known as a Zenneck wave) can be excited at the interface between two distinct dielectrics both having positive real parts of the dielectric constants. In what follows we assume that one dielectric is lossless $\varepsilon_d > 0$, while another is a high-k lossy dielectric $\varepsilon_m = \varepsilon'_m + i\varepsilon''_m$, where, additionally, $\varepsilon'_m \gg \varepsilon_d$. One can then directly use the expressions for the modal effective refractive index 4.17 and modal extents into the dielectric materials (Equation 4.19), while choosing the signs of the transverse wavevectors in both media to satisfy the surface-bounded wave condition (Equation 4.18). Resultant expressions can be further simplified in the limit $\varepsilon''_m \ll \varepsilon'_m$, which is the case for most high-k dielectrics to obtain the following expressions for the modal propagation distance (limited by material losses), and modal extents into the two dielectrics:

$$n_{eff} \underset{\varepsilon''_m \ll \varepsilon'_m}{\approx} \sqrt{\frac{\varepsilon_d \varepsilon'_m}{\varepsilon_d + \varepsilon'_m}} \left(1 + i \frac{\varepsilon_d \varepsilon''_m}{2\varepsilon'_m(\varepsilon_d + \varepsilon'_m)} \right) \underset{\varepsilon_d \ll \varepsilon'_m}{\approx} n_d - \frac{n_d^3}{2\varepsilon'_m} + i \frac{n_d^3 \varepsilon''_m}{2(\varepsilon'_m)^2} \quad (4.27)$$

$$L_d \underset{\varepsilon''_m \ll \varepsilon'_m}{\approx} \frac{\lambda}{\pi} \frac{\sqrt{\varepsilon_d}}{\varepsilon'_m} \left(1 + \frac{\varepsilon'_m}{\varepsilon_d} \right)^{\frac{3}{2}} \underset{\varepsilon_d \ll \varepsilon'_m}{\approx} \frac{\lambda}{\pi} \frac{(\varepsilon'_m)^{\frac{3}{2}}}{\varepsilon''_m \varepsilon_d} \quad (4.28)$$

$$L_m \underset{\varepsilon''_m \ll \varepsilon'_m}{\approx} \frac{L_d}{2 + \varepsilon'_m / \varepsilon_d} \underset{\varepsilon_d \ll \varepsilon'_m}{\approx} L_d \frac{\varepsilon_d}{\varepsilon'_m} \ll L_d \quad (4.29)$$

$$L_x \underset{\varepsilon''_m \ll \varepsilon'_m}{\approx} L_d \sqrt{\frac{\varepsilon'_m}{\varepsilon_d}} \gg L_d \quad (4.30)$$

From these expressions we note that, in the case of high-k dielectrics, $\varepsilon'_m \gg \varepsilon_d$, the Zenneck wave is well-defined as its propagation distance is much larger than the modal extents into both dielectrics $L_x \gg L_{m,d}$. In this limit Zenneck waves are also known as Brewster waves [41]. At the same time, modal extent into the high-k dielectric is much smaller than that into the lossless dielectric $L_m \ll L_d$. At the same time, achieving strong confinement of Zenneck waves near the surface is somewhat problematic due to inverse dependence of its transverse size on the loss of a high-k dielectric. Nevertheless, as it follows from the further analysis of Equations 4.28, 4.17, and 4.19 by using high-k dielectrics with high material losses $\text{Im}(\varepsilon_m) \sim \text{Re}(\varepsilon_m)$ allows modal size L_d in the $2\lambda - 10\lambda$ range, thus making lossy high-k dielectrics viable candidates for surface wave excitation.

4.5.5 Summary of surface waves and their classification

Here we summarise the optical properties and classify the surface waves presented so far (classification and naming convention follows that of [41]). To simplify presentation, we define $\lambda_d = \lambda/\sqrt{\epsilon_d}$ to be the wavelength of light in the lossless dielectric. In Figure 4.6 we plot the value of the surface wave relative extent into dielectric L_d/λ_d calculated using Equations 4.17 and 4.19 as a function of the normalized real and imaginary parts of the material dielectric constant ($\text{Re}(\epsilon_m)/\epsilon_d, \text{Im}(\epsilon_m)/\epsilon_d$).

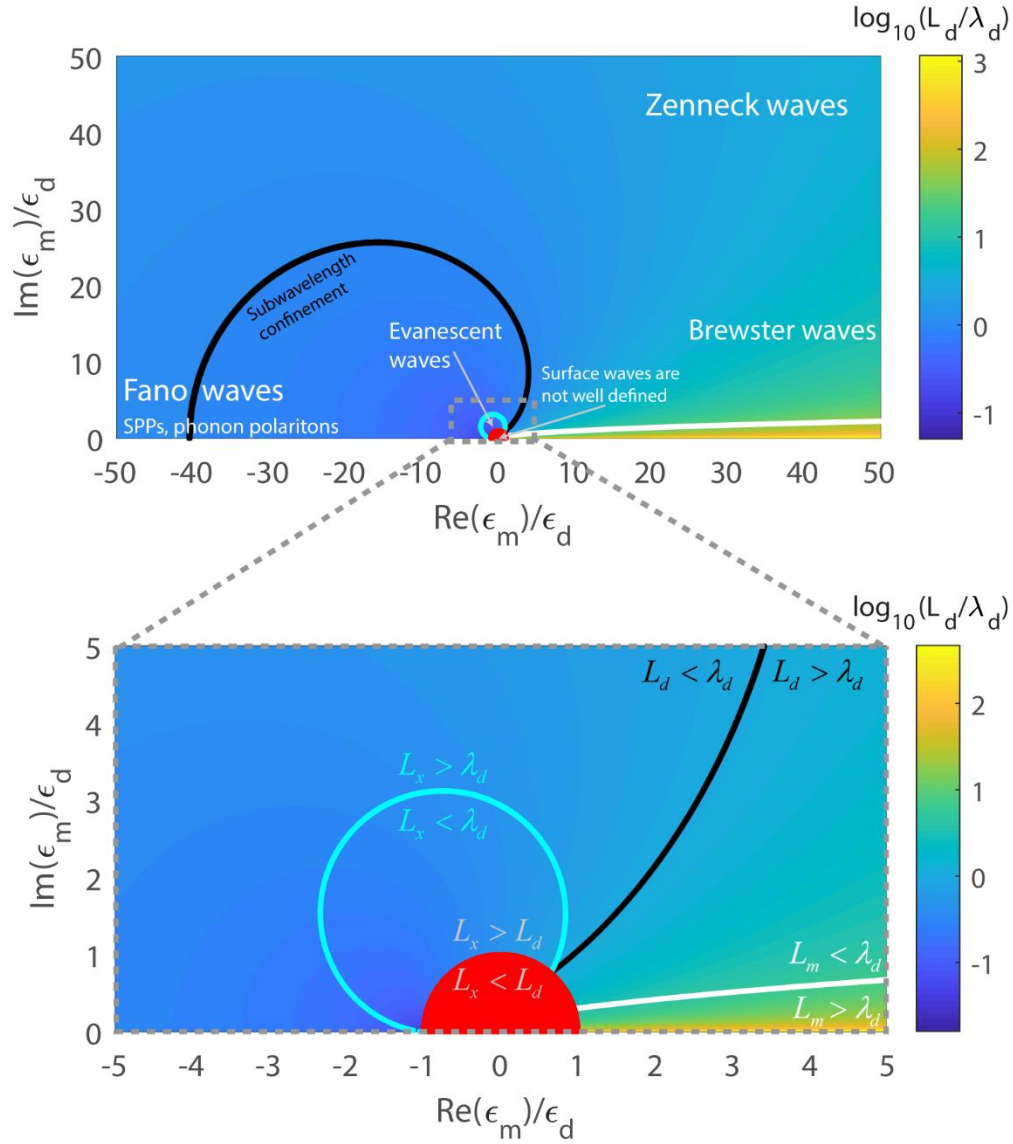


Figure 4.6 Classification of the surface waves and summary of their optical properties as a function of the complex value of the material dielectric constant ($\text{Re}(\epsilon_m)/\epsilon_d, \text{Im}(\epsilon_m)/\epsilon_d$), assuming that

the bordering dielectric (analyte) has a purely real positive dielectric constant ε_d . Plotted is the relative value of the surface wave probing depth into the dielectric (analyte), L_d/λ_d , where λ_d is the wavelength of light in the material, $\lambda_d = \lambda/\sqrt{\varepsilon_d}$. The plot is universal in these normalised coordinates.

We first note that for any choice of the material dielectric constant ε_m one can show that the surface wave penetration into material is always smaller than the surface wave penetration into dielectric $L_m < L_d$. Furthermore, in Figure 4.6 we show a black solid line that separates the regime of subwavelength confinement $L_d < \lambda_d$ from the regime of super-wavelength confinement $L_d > \lambda_d$; here we note that subwavelength confinement is achieved within a certain bounded region of absolute values of the material dielectric constant $1 < |\varepsilon_m/\varepsilon_d| < 50$. Additionally, inside a red region near the origin (dielectric constant values $|\varepsilon_m/\varepsilon_d| < 1$) surface waves are not well defined as their propagation distance along the surface becomes smaller than their extent into dielectric $L_x < L_d$, while outside of the red zone, surface waves are well-defined in the sense $L_x > L_d$.

Now we consider the regime of $\text{Re}(\varepsilon_m) < -\varepsilon_d$ and $\text{Im}(\varepsilon_m) \ll \text{Re}(\varepsilon_m)$ where Fano-type surface waves can be excited that correspond to classical surface plasmon polaritons and surface phonon polaritons. Surface plasmon polaritons of this type are typically observed in the visible and near-IR spectral range using simple metals, while at lower frequencies (THz, microwaves) one has to resort to semiconductors to excite this type of a wave. Surface phonon polaritons of this type can be observed in the mid-IR and lower frequencies (THz, microwaves) using various types of polaritonic (ex. ferroelectrics) materials. In this regime both sub- and super-wavelength probing depths into dielectric are possible depending on the value of the negative real part of the material dielectric constant. In this regime, the probing depth into the material is deeply subwavelength, $L_m \ll \lambda_d$.

Next, we consider the regime of $\text{Re}(\varepsilon_m) > 0$ and $\text{Im}(\varepsilon_m) \gg \text{Re}(\varepsilon_m)$ where Zenneck-type surface waves can be excited. Many practical materials that support Zenneck waves also feature high conductivities so that $\text{Im}(\varepsilon_m) \gg \varepsilon_d$. In this regime the probing depth into dielectric of Zenneck waves is typically significantly super-wavelength, $L_d \gg \lambda_d$, while their penetration into the material is deeply subwavelength, $L_m \ll \lambda_d$. In fact, from Figure 4.6 we note that from the point of view of surface wave confinement, there is no conceptual difference between classic Zenneck

waves and the waves excited on materials with negative value of the dielectric constant $\text{Re}(\varepsilon_m) < 0$, as long as $\text{Im}(\varepsilon_m) \gg \text{Re}(\varepsilon_m)$, and $\text{Im}(\varepsilon_m) > 30$. This type of surface waves can be observed at lower frequencies (THz, microwaves, radio waves), for example, in materials featuring high electronic conductivity (simple metals in THz and microwaves, Earth as a conductive ground for radio waves).

Then, we consider the regime of $\text{Re}(\varepsilon_m) > 0$ and $0 < \text{Im}(\varepsilon_m) \ll \text{Re}(\varepsilon_m)$ where Brewster-type surface waves can be excited. In this regime surface wave probing depth into dielectric can become super-wavelength, $L_m > \lambda_d$ (located below white solid line in Figure 4.6). Additionally, in the case of lossy high-k dielectrics featuring $\text{Re}(\varepsilon_m) \gg \varepsilon_d$, $\text{Im}(\varepsilon_m) \gg \varepsilon_d$, the probing depths into the dielectric are somewhat super-wavelength, $L_d > \lambda_d$, while their penetration into the material are weakly subwavelength, $L_m < \lambda_d$.

Finally, another interesting regime (located within a cyan circle in Figure 4.6) is near the origin where evanescent waves can be excited. These surface waves are well defined as their propagation length can be much longer than their extent into the dielectric, $L_x > L_d$, while at the same time both the modal extent into dielectric, as well as modal propagation length, are subwavelengths $L_d \ll \lambda_d$, $L_x < \lambda_d$.

4.6 Sensor sensitivities

We now derive expressions for the sensor sensitivities for the amplitude and phase sensor modalities when using various types of surfaces waves. For completeness, we also present expressions for the modal probing depths into dielectric L_d , as well as modal propagation length L_x .

4.6.1 Plasmon polaritons on simple metals

In the THz spectral range for most simple (Drude) metals $\omega \ll \gamma$, and their dielectric constant (Equation 4.20) is almost purely imaginary $\varepsilon_m'' \gg |\varepsilon_m'|$, thus:

$$\varepsilon_m(\omega) = \varepsilon_m' + i\varepsilon_m'' \approx -\frac{\omega_p^2}{\gamma^2} + i\frac{\omega_p^2}{\gamma\omega} \quad (4.31)$$

Additionally, for most analytes in the THz spectral range $\varepsilon_d \ll |\varepsilon_m'|$ and, in this limit, the effective refractive index of the surface wave given by Equation 4.17 becomes:

$$n_{eff}(n_d)_{\varepsilon_m'' \gg |\varepsilon_m'| \gg \varepsilon_d} \approx n_d - \frac{n_d^3 \varepsilon_m'}{2(\varepsilon_m'')^2} + i \frac{n_d^3}{2\varepsilon_m''} \quad (4.32)$$

while modal probing depth into the dielectric and modal propagation length are:

$$L_d_{\varepsilon_m'' \gg |\varepsilon_m'| \gg \varepsilon_d} \approx \frac{\lambda}{\sqrt{2\pi}} \frac{\sqrt{\varepsilon_m''}}{\varepsilon_d} \quad (4.33)$$

$$L_x_{\varepsilon_m'' \gg |\varepsilon_m'| \gg \varepsilon_d} \approx \frac{\lambda}{\pi} \frac{\varepsilon_m''}{n_d^3} \quad (4.34)$$

Then, by substituting Equation 4.32 into the expressions for the amplitude (Equation 4.6) and phase (Equation 4.11) sensitivities we get for plasmon polariton waves on simple metals in the THz spectral range:

$$S^A \left[\frac{1}{RIU} \right]_{\varepsilon_m'' \gg |\varepsilon_m'| \gg \varepsilon_d} \approx \frac{6}{n_d} \quad (4.35)$$

$$S^P \left[\frac{rad}{RIU} \right]_{\varepsilon_m'' \gg |\varepsilon_m'| \gg \varepsilon_d} \approx \frac{\varepsilon_m''}{n_d^3} \approx \pi \left(\frac{L_x}{\lambda} \right) \approx 2\pi^2 n_d \left(\frac{L_d}{\lambda} \right)^2 \quad (4.36)$$

We note that while amplitude sensitivity of the THz surface plasmon-polariton sensors is mostly frequency independent, their phase sensitivity is strongly frequency dependent and scale proportionally to the square of the wave probing depth L_d into the analyte.

4.6.2 Phonon-polaritons on polar materials, and plasmon polaritons on semiconductors and zero-gap materials

In addition to simple metals, plasmon-polaritons can also be excited at the interface with a semiconductor or a zero-gap material, while phonon-polariton can be excited at the interface with a polar material as long as $\varepsilon_m' < 0$, and $|\varepsilon_m'| > \varepsilon_d$. In this general case, material dielectric constant is often characterized by mostly real negative dielectric constant $\varepsilon_m'' \ll |\varepsilon_m'| - \varepsilon_d$, and in this limit the effective refractive of a surface wave is given by:

$$n_{eff}(n_d)_{\varepsilon_m'' \ll |\varepsilon_m'| - \varepsilon_d} \approx n_d - \frac{n_d^3 \varepsilon_m'}{2(\varepsilon_m'')^2} + i \frac{n_d^3}{2\varepsilon_m''} \quad (4.37)$$

while modal probing depth into the dielectric and modal propagation length are:

$$L_d_{\varepsilon_m'' \ll |\varepsilon_m'| - \varepsilon_d} \approx \frac{\lambda}{2\pi n_d} \left(\frac{|\varepsilon_m'|}{\varepsilon_d} - 1 \right)^{\frac{1}{2}} \quad (4.38)$$

$$L_x \Big|_{\varepsilon_m'' \ll |\varepsilon_m'| - \varepsilon_d} \approx \frac{\lambda}{\pi} \frac{\sqrt{|\varepsilon_m'|}}{\varepsilon_m''} \left(\frac{|\varepsilon_m'|}{\varepsilon_d} - 1 \right)^{\frac{3}{2}} \quad (4.39)$$

and the sensitivities for the two sensor modalities are then given by:

$$S^A \left[\frac{1}{RIU} \right] \Big|_{\varepsilon_m'' \ll |\varepsilon_m'| - \varepsilon_d} \approx \frac{6}{n_d} \frac{|\varepsilon_m'|}{|\varepsilon_m'| - \varepsilon_d} \quad (4.40)$$

$$S^P \left[\frac{rad}{RIU} \right] \Big|_{\varepsilon_m'' \ll |\varepsilon_m'| - \varepsilon_d} \approx \frac{1}{n_d^3} \frac{(\varepsilon_m')^2}{\varepsilon_m''} \quad (4.41)$$

We note that both amplitude and phase sensitivities of thus described THz surface plasmon-polariton and surface phonon-polariton sensors can be strongly frequency dependent, especially in the vicinity of plasmon/phonon-polariton cutoff frequencies at which $\varepsilon_m' + \varepsilon_d = 0$.

4.6.3 Zenneck waves

Finally, at the interface with a high-k dielectric ($\varepsilon_m' > 0$) for which $\varepsilon_m'' \ll \varepsilon_m'$, we use expressions presented in Section 3.4 for the Zenneck wave effective refractive index, modal probing depth into the dielectric, and modal propagation length to obtain the following sensitivities for the two sensor modalities:

$$S^A \left[\frac{1}{RIU} \right] \Big|_{\varepsilon_m'' \ll \varepsilon_m'} \approx \frac{6}{n_d} \frac{\varepsilon_m'}{\varepsilon_m' + \varepsilon_d} \Big|_{\varepsilon_d \ll \varepsilon_m'} \approx \frac{6}{n_d} \quad (4.42)$$

$$S^P \left[\frac{rad}{RIU} \right] \Big|_{\varepsilon_m'' \ll \varepsilon_m'} \approx \frac{1}{n_d^3} \frac{(\varepsilon_m')^2}{\varepsilon_m''} \Big|_{\varepsilon_d \ll \varepsilon_m'} \approx \pi \left(\frac{L_x}{\lambda} \right) \propto \left(\frac{L_d}{\lambda} \right) \quad (4.43)$$

We note that while amplitude sensitivity of the THz Zenneck wave on high-k dielectric sensors is mostly frequency independent, their phase sensitivity can be strongly frequency dependent and generally scale proportionally to the wave probing depth L_d into the analyte (as both S^P and L_d are proportional to $\varepsilon_m'/\varepsilon_m''$).

4.7 Review of materials, corresponding surface waves, and sensor performance

In what follows, we review major classes of materials that support surface waves at THz frequencies and study their potential for sensing applications. We concentrate mostly on the

uniform homogeneous materials which are the simplest to process and shape into desired devices, while only mentioning artificially structured materials in passing.

4.7.1 Simple metals

First, we consider simple metals which are mainly used in the fabrication of SPR sensors operating in the visible and IR spectral ranges [90]. As an example, in Figure 4.7 we plot properties of a surface plasmon polariton propagating at the gold/gaseous analyte ($n_d = 1$) interface in the THz spectral range and observe that while the surface state shows very low loss (long propagation distances) $L_x \gg \lambda$, at the same time, it is highly delocalized into the dielectric material $L_d \gg \lambda$. In fact, the probing depth of a surface wave into gaseous analyte can be as high as ~ 10 cm, thus making such sensors sensitive to the “bulk” changes in the analyte refractive index. Here, we used $\omega_p = 2\pi \times 2175$ THz and $\gamma = 2\pi \times 6.48$ THz for gold [42].

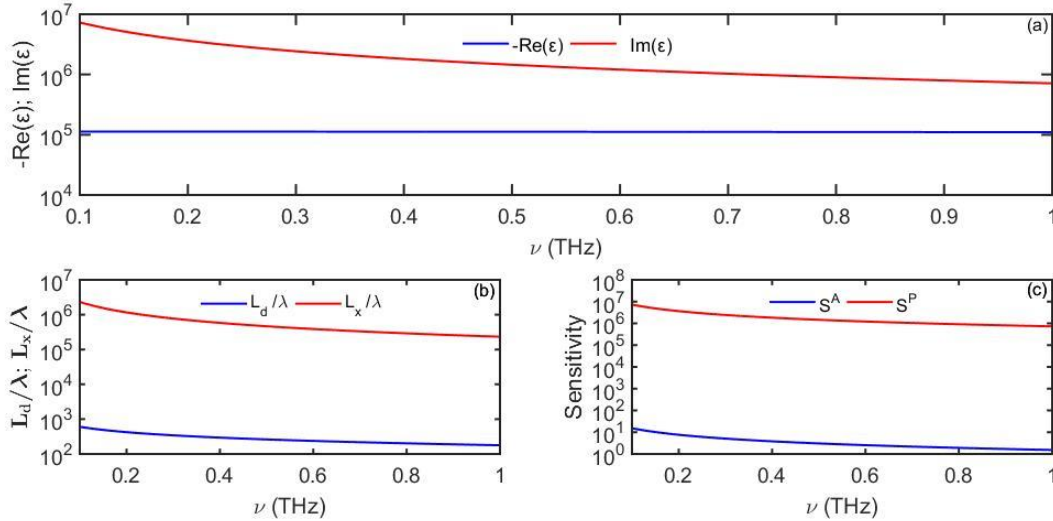


Figure 4.7 (a) Complex dielectric function of gold following the Drude model. (b) Plasmon penetration depth into the analyte and propagation distance. (c) Amplitude-based sensitivity S^A (1/RIU) and phase-based sensitivity S^P (rad/RIU) as a function of frequency. For the analyte we use $n_d = 1$.

We observe that in theory a phase-based sensor using gold as a functional material can be very sensitive to changes in the refractive index of analyte mainly due to low-loss of a surface plasmon, and as a consequence, very long sensor lengths. However, to achieve such high sensitivities as

predicted by Equation 4.36, THz plasmon-polaritons must propagate along the gold-dielectric interface for up to the theoretical propagation length of $\sim 10\text{--}100\text{ m}$. It is important to note that the experimental values of the plasmon propagation lengths along planar gold interfaces are in fact few orders of magnitude smaller than the predicted theoretical values based on the Drude model [91]. This is to be expected as the model mostly describes bulk optical properties of simple metals, while conductive surfaces might demonstrate additional phenomena not captured by the Drude model [92-95], such as surface structure modification due to atomic surface reconstruction, oxidation, pollutants, etc., as well as additional scattering losses due to geometrical imperfections at the metal surfaces, such as roughness, clustering, etc. These effects tend to increase scattering losses at the metal surface, thus leading to smaller plasmon propagation lengths and lower sensitivities of sensors based on SPPs.

4.7.2 Semiconductors

Next, we consider semiconductor materials which are directly analogous to simple metals and can often be described using a Drude model (Equation 4.20). However, plasma frequency of semiconductor materials generally expressed as:

$$\omega_p = \sqrt{\frac{e^2 N}{\epsilon_0 m^*}} \quad (4.44)$$

is generally significantly lower than that of the simple metals (and can even be pushed into the THz spectral range) due to lower concentrations of the free carriers N . We are particularly interested in materials that have plasma frequency in the THz spectral range, while also having relatively small absorption loss so that $\epsilon'_m + \epsilon_d < 0$ and $\epsilon''_m \ll |\epsilon'_m| - \epsilon_d$. Under these conditions (see Section 4.6.2), such materials can support tightly localized surface states in the THz band that are directly analogous to plasmon polaritons in the visible spectral range.

As an example, consider InSb, a semiconductor with plasma frequency of 7.32 THz that can support highly localized surface plasmon-polariton modes [96]. In the THz spectral range it presents a great alternative to simple metal as it can be used to create waveguides and SPR sensors using industrial microfabrication process [80, 97]. Moreover, its free carrier concentration (and, hence, surface wave optical properties) can be adjustment via temperature tuning and doping. Additionally, magnetic fields can be utilized to modulate electrical and optical proprieties of this magneto-optical material [98], thus enabling new sensor modalities.

Another example is an *n*-type and a *p*-type GaAs films produced by using two different doping types as reported [99] (Drude parameters are summarized in the Table 4.1).

Tableau 4.1 Drude parameters for the *n*-type and *p*-type GaAs films.

GaAs	$m^* (m_0)$	$N (\text{cm}^3)$	$\tau (\text{s})$	$\omega_p/2\pi (\text{THz})$	$\gamma/2\pi (\text{THz})$
<i>n</i> -type	0.079	4.48×10^{18}	8.47×10^{-14}	67.62	1.879
<i>p</i> -type	0.34	1.15×10^{18}	2.51×10^{-14}	16.51	6.341

In Figure 4.8 we present the complex dielectric function for the *n*-type and *p*-type GaAs films along with the expected plasmon propagation length and penetration depths into the analyte. We observe that the surface wave penetration depth into the analyte is smaller for the *p*-type (that has plasma frequency closer to the terahertz spectral range) than for the *n*-type. At the same time, more tightly localized surface waves propagating on the *p*-type semiconductor are lossier than those propagating on the *n*-type one, consequently, their phase sensitivity is smaller compared to that of the surface waves propagating on the *n*-type semiconductor, a behavior that is consistent with that of simple metals (see Equation 4.36). We, thus, conclude that doping could be used as a design parameter to tune the surface wave probing depth into the analyte depending on the desired sensor application.

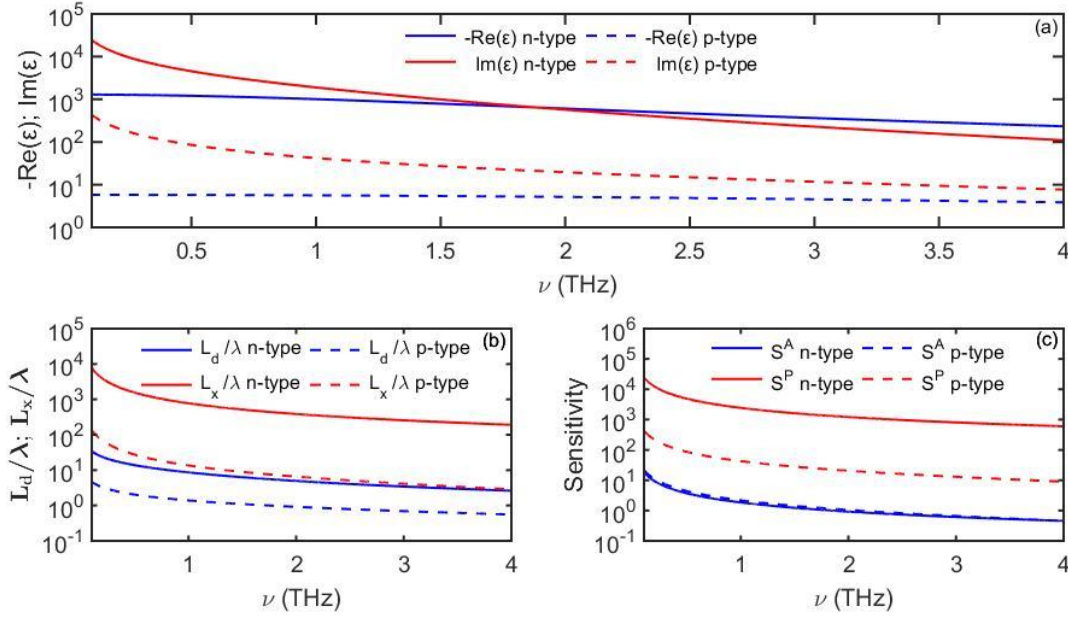


Figure 4.8 (a) Dielectric function of the *n*-type and *p*-type GaAs films following Drude model (Table 4.1). (b) Plasmon penetration depth into the analyte and propagation distance. (c) Amplitude-based sensitivity S^A (1/RIU) and phase-based sensitivity S^P (rad/RIU) as a function of frequency. For the analyte we use $n_d = 1$.

4.7.3 Polar materials

Now, we consider polar materials, which are characterized by the complex dielectric permittivity that also depends on the intermolecular and intramolecular resonance frequencies. The Lorentz model is typically used to model the frequency response of the dielectric function of polar materials [100]:

$$\epsilon(\omega) = \epsilon_\infty \left[1 - \frac{\omega_p^2}{\omega^2 - \omega_0^2 + i\gamma\omega} \right] \quad (4.45)$$

where ϵ_∞ is the dielectric constant at high frequency, ω_p is the plasma frequency, ω_0 is a resonance frequency and γ is the damping coefficient. The real and imaginary parts of the dielectric constant (Equation 4.45) can be expressed as:

$$\epsilon'(\omega) = \epsilon_\infty \left[1 - \frac{\omega_p^2(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} \right] \quad (4.46)$$

$$\epsilon''(\omega) = \frac{\epsilon_\infty \omega_p^2 \gamma \omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2} \quad (4.47)$$

For such polar materials, the real part of the permittivity can be negative near the resonance frequency $\omega > \omega_0$. As the nature of the resonance, especially at THz frequencies, is often related to the vibrational movements of macromolecules or material domains, then the resultant surface waves can be called phonon polaritons. Table 4.2 summarizes the Lorentz parameters for some polar materials:

Tableau 4.2 Lorentz parameters for various polar materials.

Material	ϵ_∞	$\omega_0/2\pi$ (THz)	$\omega_p/2\pi$ (THz)	$\gamma/2\pi$ (THz)
PVDF [101]	2.0	0.3	1.47	0.1
D-Glucose [102]	2.940	1.446	0.037	0.021
SrTiO ₃ [103]	8.528	2.632	15.77	0.6
LiNbO ₃ (ordinary) [104]	13.2	4.53	6.99	0.51
LiNbO ₃ (extraordinary) [104]	20.6	3.87	2.04	0.69
LiTaO ₃ (ordinary) [104]	13.4	4.23	6.12	0.15
LiTaO ₃ (extraordinary) [104]	8.4	5.96	11.63	0.34

In Figure 4.9 we present dielectric properties of the PVDF material along with the phonon-polariton propagation distance and penetration depth into the analyte. We observe that the surface wave confinement is more significant at higher frequencies, especially closer to the phonon-polariton cutoff frequency at which $\epsilon'_m(\omega_{cutoff}) + \epsilon_d = 0$. We also note that at frequencies right below the resonance frequency ω_0 , polar material dielectric constant can have very large and positive values of both their real and imaginary parts, which is similar to the case of lossy high-k dielectrics. As a result, immediately below the resonance frequency ω_0 , polar materials support Zenneck waves, while above the resonance frequency ω_0 they support phonon polaritons. We also observe that the surface wave probing depth into the analyte is subwavelength for the most part of the THz frequency range, thus enabling “surface” sensing with surface phonon polaritons.

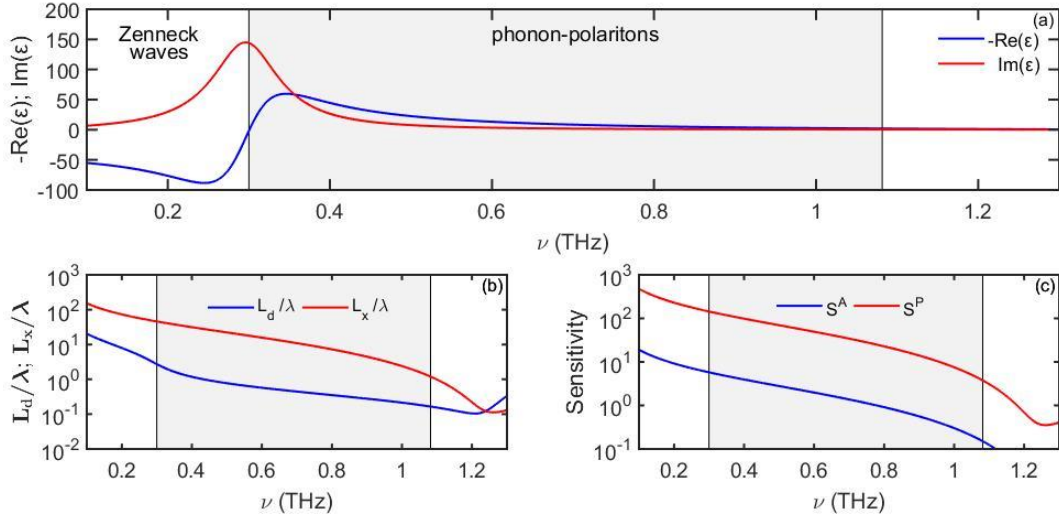


Figure 4.9 (a) Dielectric function of PVDF following Lorentz's model. (b) Phonon-polariton penetration depth into the analyte and propagation distance. (c) Amplitude-based sensitivity S^A (1/RIU) and phase-based sensitivity S^P (rad/RIU) as a function of frequency. For the analyte we use $n_d = 1$.

4.7.4 Zero-gap materials

Zero-gap materials are semiconductors where the conduction and valence band edges meet at the Fermi level [105]. Here, the electrons can easily change state to fill empty bands. Therefore, these materials are extremely sensitive to external influences such as pressure and magnetic field. Graphene, which consists of a 2D hexagonal arrangement of carbon atoms, is a famous example of a zero-gap semiconductor. This material, which can be tuned by a magnetic field and chemical doping, which could lead to the development of many new electronic devices [106]. The dielectric function of a monolayer of graphene is given by [107]:

$$\tilde{\epsilon}(\omega) = 1 - \frac{1}{\pi \hbar^2 \epsilon_0 t_g} \frac{e^2 \mu}{\omega(\omega + i\tau^{-1})} \quad (4.48)$$

where $t_g = 0.34$ nm is the thickness of the graphene monolayer, μ is the chemical potential and τ is the scattering rate. In Figure 4.10 we plot the dielectric properties in the THz spectral range of a doped monolayer graphene film of $\mu = 0.135$ eV and $\tau = 1.35 \times 10^{-13}$ s [108]. In contrast to simple metals, real part of the graphene dielectric constant is larger (in absolute value) than its

imaginary part for most of the THz spectral range. Here, the plasmon-polariton confinement increases with frequency and modal size becomes comparable with the wavelength at higher frequencies (~ 3 THz). Due to a significant modal penetration depth into the analyte, plasmon-polariton loss is low, thus resulting in very long plasmon propagation distances.

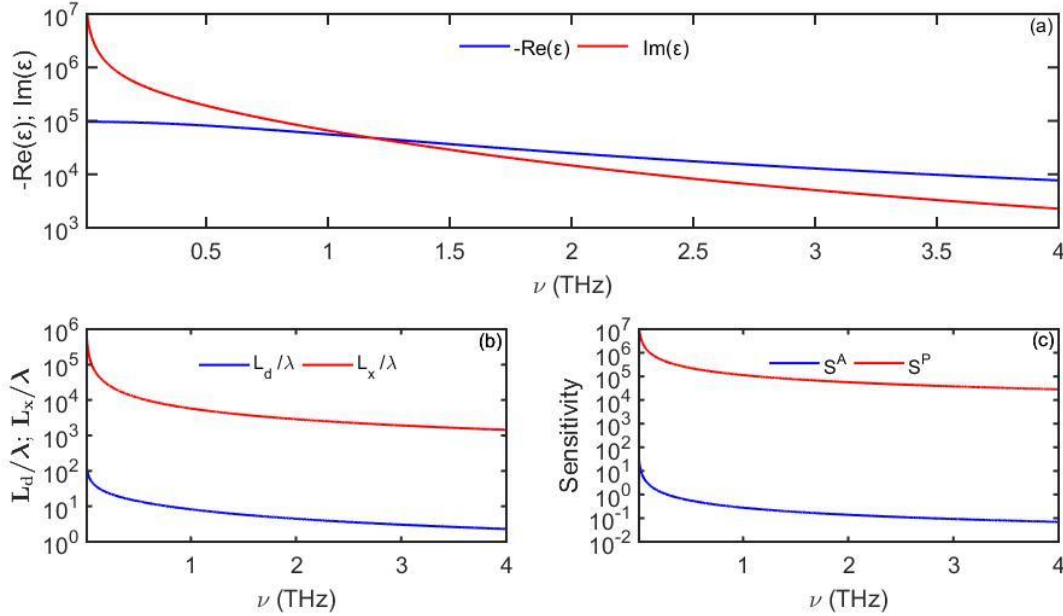


Figure 4.10 (a) Dielectric function of a doped monolayer of graphene. (b) Plasmon penetration depth into the analyte and propagation distance. (c) Amplitude-based sensitivity S^A (1/RIU) and phase-based sensitivity S^P (rad/RIU) as a function of frequency. For the analyte we use $n_d = 1$.

4.7.5 Lossy high-k dielectrics

In Section 4.5.4 we demonstrated that a well-defined surface wave can propagate at the surface of a lossy high-k dielectric. In particular, to support a well-localized surface mode one has to require that the imaginary part of the high-k dielectric constant is comparable to its real part. As an example, in Figure 4.11 we present optical properties of a $0.4\text{Ba}_{0.6}\text{Sr}_{0.4}\text{TiO}_3\text{-}0.6\text{La}(\text{Mg}_{0.5}\text{Ti}_{0.5})\text{O}_3$ (BST-LMT) ceramic as reported [109], as well as the optical properties of a Zenneck wave that can propagate at the high-k dielectric/analyte interface. Note that in this particular example, despite the relatively large modal extent into the analyte ($L_d \sim 10\lambda$), the modal propagation length is considerably longer than the modal size ($L_x \sim 70\lambda \gg L_d$), thus a well-defined surface state is achieved at the high-k dielectric/analyte interface.

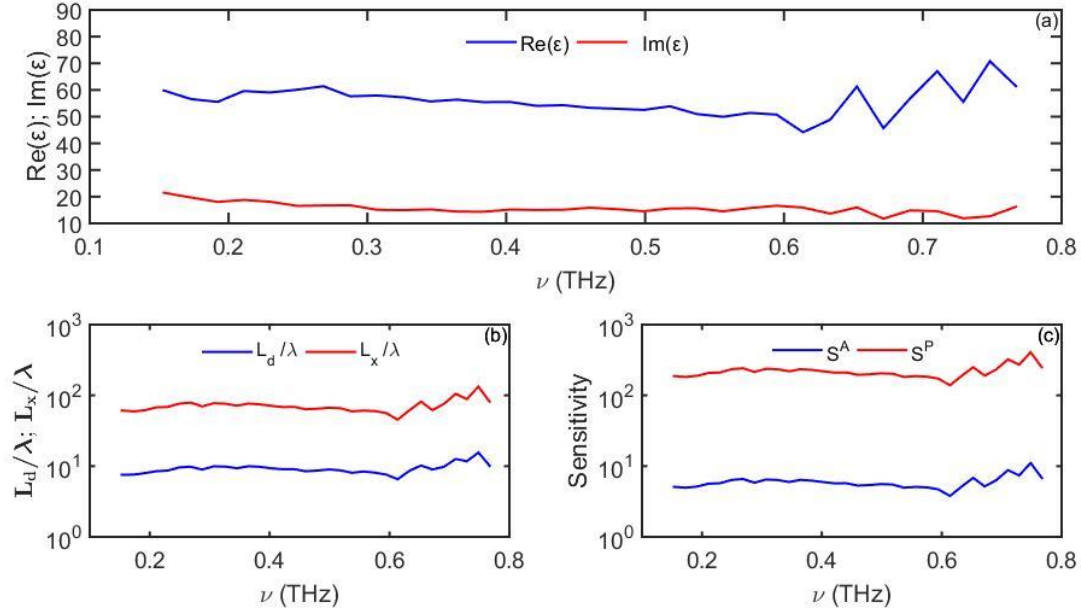


Figure 4.11 (a) Experimental values of the complex dielectric constant of a BST-LMT at room temperature. (b) Zenneck-wave penetration depth into the analyte and propagation distance. (c) Amplitude-based sensitivity S^A (1/RIU) and phase-based sensitivity S^P (rad/RIU) as a function of frequency. For the analyte we use $n_d = 1$.

More generally, high- k dielectrics are relatively abundant in the form of various oxides and ceramics, while some of them (such as TiO_2 , Zr SnTiO_3 , $\text{MgO-TiO}_2\text{-ZnO}$, $\text{Ba}_2\text{Nd}_5\text{Ti}_9\text{O}_{27}$, $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$, $\text{ZnTi}_{1-x}(\text{Al}_{0.5}\text{Nb}_{0.5})_x\text{Nb}_2\text{O}_8$, etc. [110-116]) also feature relatively high imaginary parts of their dielectric constant compared to their real parts.

4.7.6 Artificially structured materials (metamaterials)

Thus far, we have covered several types of naturally occurring homogeneous materials, such as simple metals, semiconductors, polar materials, zero-gap materials, and high permittivity materials that support various types of surface modes. At the same time, highly confined modes in terahertz range can also be obtained by using artificially structured materials [63]. One type of such structured material features a periodic array of subwavelength-size grooves inscribed onto a planar metallic slab in air. Thus, for a 1D array of grooves of width a , depth h , and lattice constant d (period), the complex dispersion relation of the fundamental surface mode supported by such a

material (also known as a spoof surface plasmon) in the limit $a\omega n_{eff}^{spoof}/(2c) \ll 1$ can be shown to be:

$$\varepsilon_{eff}^{spoof}(\omega) \approx \varepsilon_d + \left(\frac{a}{d} \frac{\tilde{\beta}_0}{k_0} \tan(\tilde{\beta}_0 h) + i \frac{\varepsilon_d}{\sqrt{\varepsilon_m}} \frac{d-a}{d} \right)^2 \quad (4.49)$$

where:

$$\tilde{\beta}_0 \approx k_0 \sqrt{\varepsilon_d} + i \frac{\sqrt{\varepsilon_d}}{a\sqrt{\varepsilon_m}} \quad (4.50)$$

and ε_m is the complex dielectric constant of a lossy metal. To derive the complex dispersion relation 4.49, one can use standard derivation together with the impedance boundary conditions at the metal surface [44]. Figure 4.12 shows complex dielectric function of the fundamental spoof surface plasmon $\varepsilon_{eff}^{spoof}$, its penetration depth into the analyte and propagation distance defined by Equation 4.19, as well as expected maximal sensitivity of an amplitude-based sensor (Equation 4.6) and a phase-based sensor (Equation 4.11) for two structured materials with the following geometrical parameters $h = d$ and $h = 2d$, where $a = d/2$ and $d = 40 \mu\text{m}$.

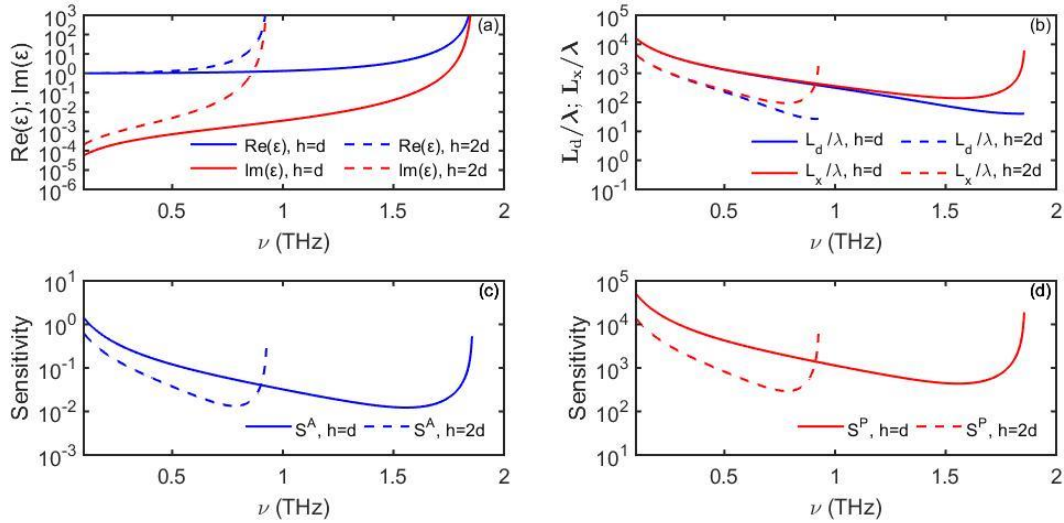


Figure 4.12 (a) Dielectric function of spoof surface waves supported by gold with periodic grooves ($a = d/2$ and $d = 40 \mu\text{m}$). (b) Spoof plasmon penetration depth into the analyte and propagation distance. (c) Amplitude-based sensitivity S^A (1/RIU) as a function of frequency. (d) Phase-based sensitivity S^P (rad/RIU) as a function of frequency. For the analyte we use $n_d = 1$.

At the macroscopic scale, this structured material (or metamaterial/effective medium) is analogous to a homogeneous medium that is able to support electromagnetic surface waves. Such a material can also be viewed as an artificial metal with a modified plasma frequency [75]. Many other structured materials were engineered to support surface plasmon-polariton-like modes, including 2D patterned and 3D patterned metals [48, 117], helically-grooved metal wires [69], as well as dielectric-based metamaterials [118]. Moreover, more exotic waves known as Dyakonov waves can be produced at the interface with anisotropic materials which, at THz frequencies, can be, for example, in the form of periodic multilayers of two different materials featuring a deeply subwavelength period [42].

4.8 Discussion

In the previous sections we reviewed several principal material types that allow excitation of the well-defined surface waves in the THz spectral range. Additionally, we have classified surface waves according to their physical nature and presented expressions for their penetration depth into the analyte, propagation length, as well as amplitude-based and phase-based sensitivities. For some of the surface wave types we also noted a correlation between the corresponding phase-based sensor sensitivity and probing depth into the analyte which, for plasmon polaritons on simple metals and some semiconductors, was $S^P \propto (L_d/\lambda)^2$, while for Zenneck waves on high-k lossy dielectrics, it was $S^P \propto L_d/\lambda$. For these wave types, sensors featuring smaller probing depths into the analyte (tighter modal confinement) also feature lower sensitivities. In other words, “surface” sensors (with subwavelength modal confinement) tend to have lower sensitivities than their “bulk” counterparts. In Figure 4.13, we summarize the article’s findings by plotting surface wave penetration depth into the analyte against the maximal sensitivity of a phase-based sensor for various types of surface waves/materials considered in this paper at a 1 THz operation frequency.

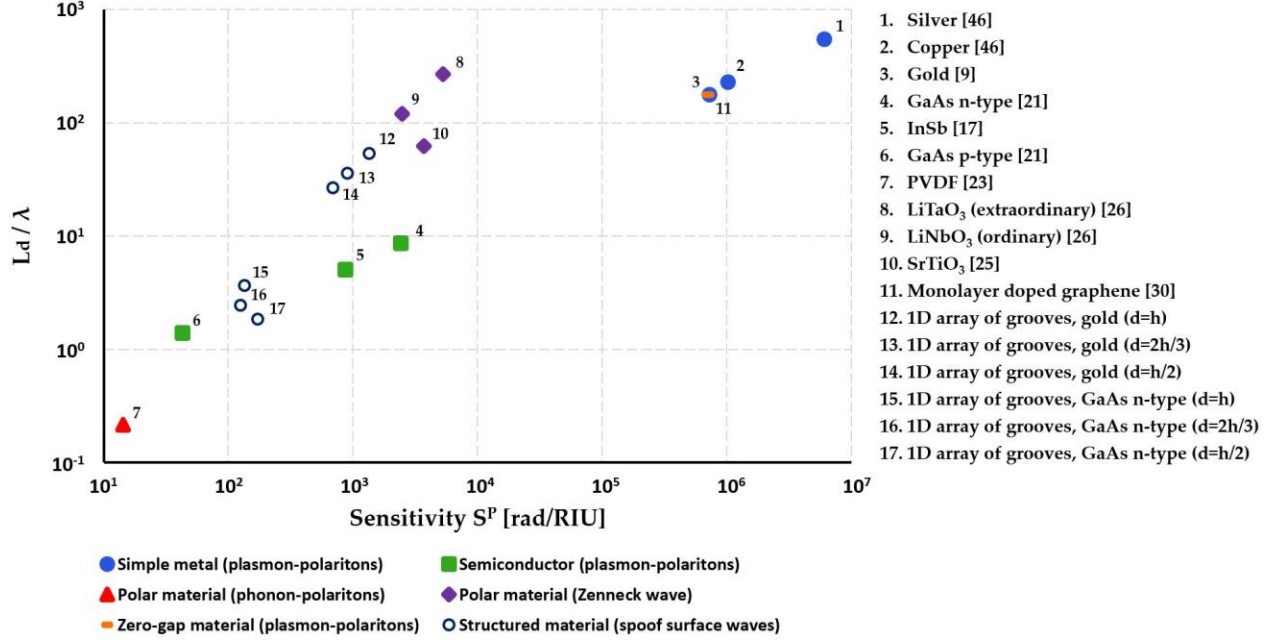


Figure 4.13 Surface wave penetration depth into the analyte against the maximal sensitivity of a phase-based sensor for various types of surface waves/materials considered in this paper at a 1 THz operation frequency. For structured materials we use $a = d/2$, $d = 40 \mu\text{m}$. For the analyte we use $n_d = 1$. Silver and copper optical properties [119].

We can also define sensors with modal probing depth into the analyte above ~ 10 wavelengths as “bulk” sensors, while those with smaller modal sizes are defined as “surface” sensors. Thus, the main candidates as enabling materials for THz surface sensing are semiconductors with plasma frequencies in the THz range, polaritonic materials with resonance frequencies in the THz spectral range, or structured materials that support THz spoof plasmons, and they are capable of phase sensitivities in the $10\text{--}10^4$ rad/RUI range and require relatively small sensor sizes (short modal propagation length). Higher phase sensitivities $10^4\text{--}10^7$ rad/RUI can be achieved using simple metals, zero-gap materials, semiconductors with high plasma frequency, lossy high-k dielectrics, and some structured materials, however, they operate in the bulk sensing modality with penetration depth as high as $10^2\text{--}10^3 \lambda$, and often require large sensor sizes (long modal propagation length). Thus, depending on the sensor application modality, size limitation, and required sensitivity, a judicious choice of the surface wave type and enabling material has to be made.

It is important to note that optical properties of the surface waves are extremely sensitive to the surface preparation and presence of both material and geometrical imperfections at the interface [90, 91]. Therefore, one has to be conscious that theoretical estimates presented in this paper for the wave optical properties and sensor sensitivities can be significantly different from the experimental ones. Additionally, one must be aware that different surface preparations of even the same material samples can result in significantly different optical properties of the surface waves.

We also note that in this paper we only aim at highlighting and comparing different types of “pure” surface waves that propagate along ideal planar surfaces. Clearly, optical properties of such waves can be significantly modified and augmented (lower losses, stronger confinement near the surface, etc.) when using even the simplest surface modification techniques, such as the deposition of judiciously chosen subwavelength-size dielectric layers [120, 121], etc. Such techniques are important and diverse and deserve a review paper of their own.

Finally, we would like to discuss briefly an issue of excitation of the THz surface waves. Efficient excitation is generally a challenging task due to the mismatch of the propagation constants of the incident waves (which are typically launched from the side of an analyte) with that of a surface wave. Additionally, there is also an issue of spatial field matching complicated by the strong spatial inhomogeneity of the surface waves in the direction perpendicular to the interface. The simplest methods for surface wave excitation employs strongly spatially inhomogeneous fields near the interface, thus generating both propagating and evanescent fields in the near vicinity of the surface. While some of these waves can couple to the surface waves, most are lost to radiation, thus resulting in the relatively low efficiency coupling with the main advantage being simplicity of the coupling arrangement. As an example, aperture-limited plane wave has been studied in great details and used for the excitation of SPPs and Zenneck waves [120, 122]. Strongly inhomogeneous fields near the interface can be obtained by using a short parallel plate waveguide parallel to the surface [121] or even a simple end-fire (butt coupling) arrangement where an incident electromagnetic field is focused onto the input facet at the position of the material/analyte interface [123]. Other methods that typically result in higher excitation efficiency of surface waves rely on careful matching of the wavevectors of an incident wave (normally from the side of an analyte) with that of a surface wave, while also employing some type of a directional coupler arrangement. A classic technique based on this principle employs a higher refractive index (compared to that of an analyte) prism coupler, where the incident angle of the excitation wave is chosen in such a way as to match the propagation

constant of the incident wave (projection of the wavevector onto the surface plane) with that of a surface wave [124]. Another classic technique achieves matching of the excitation field and surface wave propagation constants by employing diffraction grating inscribed onto the surface [58]. A more exotic surface wave excitation scheme uses frequency difference generation of THz radiation near the metalized surface of a nonlinear material by employing two slightly mismatched in frequency IR lasers [125, 126]. The generation of surface waves is obtained when both the wavevector and energy conservation conditions are respected between two IR laser waves and a THz surface wave. Finally, in addition to many of the methods mentioned above, excitation of surface waves on structured surfaces (spoof plasmons) was achieved by coupling to traditional waveguides via tapers or mode converters [127].

4.9 Conclusions

In this paper we reviewed two major types of sensor detection modalities (amplitude-based and phase-based) in the context of the surface wave enhanced sensing in the terahertz frequency band. A variety of surface wave types were considered including surface plasmon polaritons on metals, semiconductors, and zero gap materials, surface phonon polaritons on polaritonic materials, Zenneck waves on high-k dielectrics, as well as spoof surface plasmons and spoof Zenneck waves on structured interfaces. Special attention was paid to the tradeoff between surface wave localization and sensor sensitivity. Furthermore, a detailed theoretical analysis of the surface wave optical properties as well as the sensitivity of sensors based on such waves was supplemented with many examples related to naturally occurring and artificial materials.

Author contributions

Writing, Mathieu Poulin and Maksim Skorobogatiy; Contribution in Lossy High-k Dielectrics section and review, Steven Giannacopoulos. All authors read and approved the final manuscript.

CHAPITRE 5 ARTICLE 2 : SPOOF SURFACE WAVES ON NON CONDUCTING STRUCTURED INTERFACES

Le deuxième article fait suite à la revue de littérature précédente, où une solution pour le support de modes de surface dans la gamme spectrale des térahertz est proposée. Ici, l'utilisation d'un matériau structuré capable de localiser l'énergie dans ces interstices au lieu d'un matériau homogène offre la possibilité de supporter des modes de surface ayant des propriétés similaires aux ondes de surface analogues retrouvées dans les plages spectrales de l'infrarouge et du visible. De plus, contrairement aux structures métalliques qui ont déjà été étudiées par la communauté scientifique pour le support de modes de surface térahertz, le métamatériau proposé est non conducteur, impliquant que le matériau hôte ne peut pas être approximé par un conducteur électrique parfait. Une dérivation des équations de Maxwell pour ce problème est donc nécessaire afin de retrouver une relation de dispersion pour ce nouveau type de mode de surface supporté par des matériaux diélectriques structurés. Afin de simplifier le problème, le métamatériau choisi suivant la revue de littérature est une surface possédant des gravures périodiques selon une direction.

Suivant la relation de dispersion, une étude extensive des propriétés des modes de surfaces en fonction des paramètres du métamatériau est présentée. De plus, des résultats provenant de simulations numériques du problème accompagnent les valeurs analytiques afin d'illustrer la distribution du mode dans la structure ainsi que pour valider la dérivation analytique de la relation de dispersion. Enfin, des méthodes pour exciter de tels modes sont proposées. Cet article a été soumis pour une future publication dans le journal « IEEE Transactions on Antennas and Propagation ».

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5.2 Abstract

Spoof surface waves are demonstrated theoretically to propagate along periodic corrugated surfaces made of non-conductive materials with positive permittivity. An analytic derivation of the spoof surface wave dispersion relation is presented in the case of deeply subwavelength period of a corrugated structure using impedance boundary conditions at the interfaces. Thus obtained dispersion relation is verified numerically and limitations as well as physicality of impedance boundary conditions when modeling spoof surface waves are discussed. Finally, suitable materials, potential experimental realization, and sensing applications of spoof surface waves in the terahertz spectral range are discussed.

5.3 Introduction

The strong spatial confinement of surface waves near interfaces allows to greatly enhance performance of many practical devices in high-resolution sensing, spectroscopy, and subwavelength imaging [1, 6, 10, 34, 128-131]. Particularly, surface plasmon-polaritons propagation at the interface between a metal and an analyte revolutionized the field of bio-sensing in the visible spectral range [132-134]. Recently, THz (terahertz) spectral range emerged as the next frontier for non-destructive imaging and biomedical applications [13, 22-24, 75, 77, 135, 136]. Because of the relative transparency of dry dielectrics to THz radiation and existence of spectral fingerprints for many biological molecules, THz sensing became an emerging research field that could also benefit from surface wave sensing modality. However in the long wavelength spectral range, excitation and application of surface waves have been problematic due to the THz wave weak confinement (strong presence in the cladding) and high losses [42, 137]. This is because in the THz spectral range, imaginary part of the metal dielectric constant dominates and it can be several orders of magnitude larger than the real part unlike in the visible and near-IR spectral ranges, where real part of the metal dielectric constant is negative and much larger (in its absolute value) than the imaginary part. This entailed a search for new polaritonic materials capable of supporting THz surface waves with strong localisation at the interface [91, 96, 98, 101, 110, 111, 138, 139]. One interesting alternative to surface plasmon-polaritons at long wavelengths are surface phonon-polaritons, which are excited on surfaces of some polar materials, typically in the near vicinity of material optical resonances. Such surface waves is a result of coupling between phonon

and electromagnetic fields, with enabling materials abundant in the mid-IR and THz spectral ranges [97, 140] in the form of semiconductors and ceramics. Near optical material resonances, optical properties of surface phonon-polaritons in the THz spectral range can be similar to those of a surface plasmon polariton in the visible. This is because dielectric permittivity of a polaritonic material can feature a negative real dielectric constant that is much larger (in absolute value) than its imaginary part, which is similar to the case of metals in the visible and near-IR.

Recently, materials with subwavelength structuring were shown to offer an alternative to the traditional homogeneous materials for the excitation of surface waves as their interfacial optical properties are highly designable [43, 50, 52]. Specifically, in the THz spectral range, a large body of work now exists on structured interfaces that are capable of supporting surface states. Particularly, structured metallic surfaces featuring periodic sequence of narrow air-filled grooves of various geometries such as rectangular [44, 48, 62, 141], and V-shape [55, 56], along with corrugated metallic wires [68, 71], and helically grooved wires [69] were shown to support surface waves called spoof surface plasmons that feature strong field localization in the vicinity of metal, similar to the classical plasmon-polaritons from the visible spectral range. Additionally, corrugated surface made of semiconductors can also be designed to support spoof surface waves [59, 60]. In practice, however, due to high material losses of metals in the THz spectral range, and due to tight modal confinement in the narrow metallic grooves, propagation losses of these spoof surface plasmons tends to be large. One way to reduce the loss of a spoof surface wave is to push its fields out into the low-loss air cladding by either using shallow grooves [53], metallic wedges [142] or by replacing a corrugated plate with a corrugated metallic stipe [61, 64-66], in both cases, however, surface wave confinement near corrugated interface is decreased. Remarkably, spoof surface waves can also be excited on ideal lossless metallic surfaces characterized by the infinite negative dielectric constant (Perfect Electric Conductor) [45, 117, 143]. In this case, the moniker “spoof”, which is used to identify surface waves on the corrugated interfaces, has a clear logical meaning. Indeed, it identify waves that mimic the behaviour of classic surface plasmon polaritons, while propagating at the interface with a material (PEC) that does not naturally support surface waves. In this work, by analogy to the nomenclature used to identify “spoof” waves on corrugated PEC interfaces, we call “spoof” surface waves the guided modes that propagate along corrugated non-conductive interfaces. Indeed, the use of a “spoof” moniker is justified in our case as, normally,

there is no guided mode exists at the planar interface between two lossless dielectrics. It is the corrugation of such an interface that allows to support a “spoof” surface state.

However, a detailed analysis shows that to support a guided wave, it is only necessary for the underlying material to be lossy (have a non zero imaginary part of the dielectric constant), while the sign of a real part of the dielectric constant is irrelevant [41, 137]. This suggests that surface modes could also be supported by positive permittivity constant materials. The problem stems from the realisation that reliable experimental characterization of such waves normally requires their relatively strong localization at the interfaces (transverse modal sizes of several tens to hundreds of wavelengths at most) to prevent significant interaction with the environment. Moreover, it is also desirable for the surface wave propagation distances to be much longer than the wave transverse size, as in this case surface wave resembles to a guided mode that can be excited and probed much like a regular guided mode of a waveguide. Unfortunately, for many real materials and practical operation conditions, these surface waves are either extremely extended into the cladding and thus easily lost to the environment, or they feature very high transmission losses that result in the surface wave propagation length comparable to the wave transverse size. For these reasons, such surface waves are often difficult to excite and classify as true guided modes rather than some kind of local geometrical resonances. Thus, homogeneous positive permittivity materials do not correspond to a viable alternative to the various corrugated negative permittivity material such as the structured metallic surfaces for the support of surface wave in the THz spectral range.

In this paper, we demonstrate for the first time to our knowledge that the well-defined spoof surface waves can propagate on structured non-conductive surfaces made of loss-less dielectrics featuring real positive permittivity constants. Particularly, we show that using common high permittivity materials and judicious choice of the surface geometry one can realise strong confinement of spoof surface waves near the interface, as well as propagation distances that greatly exceed the wave transverse size. Moreover, under certain conditions, spoof surface waves can also propagate along structured surfaces made of a material with infinite positive dielectric constant (Perfect Isolator). More precisely, we study corrugated surfaces featuring 1D periodic arrays of grooves filled with lossless low-permittivity dielectric of the upper cladding. Such grooves are separated by notches made of high-permittivity dielectric of the lower cladding. Dispersion relation of spoof surface waves are obtained semi-analytically in the long wavelength limit by solving Maxwell equations in the vicinity of a structured surface following a general approach detailed in [44, 144]. One key

difference of our derivation compared to the ones presented in the abovementioned references is that we use impedance boundary conditions (IBC) at the interface with a structured interface, as well as positive values of the material dielectric constants [145]. This also entails an important and unique for this problem discussion about the effect of radiation leakage from the grooves into the notches, potential dissipation mechanisms of such leaked radiation inside the notches, as well as necessity for suppression of radiation-induced coupling between adjacent grooves. Semi-analytical results with IBC were then confirmed with numerical simulations using COMSOL Multiphysics Software with IBC, and very good correspondence was observed. Finally, a full simulation using COMSOL using two cladding materials and a structured interface confirmed that our semi-analytical theory indeed describes well spoof surface waves on non-conductive surfaces except for resonant frequencies at which structural resonances are excited within the high dielectric permittivity notches. In principle, such resonances can be removed by various techniques as described further in the paper. Although our derivations are not wavelength specific, without the loss of generality we present examples in the THz spectral range (0.1 to 1 THz) in view of future experimental work on optical characterization of such waves.

5.4 Analytical derivation of the dispersion relation

Consider a periodically corrugated surface made of a material with real and positive permittivity $\varepsilon_m > 0$ adjacent to a lossless dielectric filler of permittivity $\varepsilon_0 > 0$ as shown in Figure 5.1.

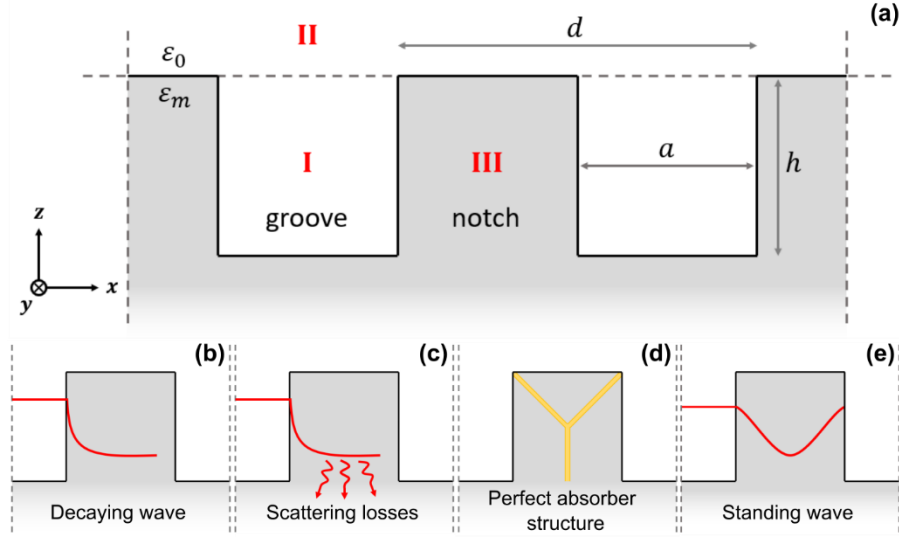


Figure 5.1 Schematic of the corrugated interface, and validity of the Impedance Boundary Condition. (a) Schematic of the corrugated interface. The period is d and the width and height of the grooves are respectively a and h . The permittivity of the dielectric filler above the corrugated surface (zones II) and in the grooves (zone I) is ϵ_0 , while permittivity of the corrugated surface (zone III) is ϵ_m . (b)-(e) Validity of the Impedance Boundary Condition demands that the outgoing wave from the interface of the grooves (into notches) is either absorbed (b) or scattered (c) or suppressed (d), (e) from interacting with other interfaces within the notches.

This periodic structure has a period d and contains grooves of width a and height h . In what follows we call notches the rectangular regions of length $d - a$ between grooves that are filled with material ϵ_m . Both materials are assumed to be non-magnetic. The dispersion relation of a spoof surface wave supported by the interface can be found by solving the Maxwell equations in the semi-infinite upper zone II ($z > 0$) and grooves in the lower zone I ($z < 0$), while respecting the continuity conditions of the fields at $z = 0$. Additionally, the impedance boundary condition is used at the interfaces with the high dielectric material (zone III) in the following form [146]:

$$\eta_s \mathbf{s} \times \mathbf{H} + \mathbf{s} \times (\mathbf{s} \times \mathbf{E}) = 0 \quad (5.1)$$

where η_s is the surface impedance and $\mathbf{s}$ is the unit normal vector to the interface. This simplest form of IBC can be derived by considering a planewave incident from the material with lower dielectric permittivity onto a planar interface with material with higher dielectric permittivity. The

incident E&M fields satisfy Equation 5.1 at the interface, assuming that only an outgoing wave is present on the side of a higher permittivity dielectric. This boundary condition is attractive in its simplicity, but if it is to be of universal nature and practical utility, it is necessary that the surface impedance η_s be independent of the incident field characteristics, such as polarization and angle of the incident plane wave. Following [146] one can demonstrate that if the two materials occupying the half spaces are homogeneous and isotropic, and if the incident wave comes from material ϵ_0 , while for the second material $|\epsilon_m| \gg \epsilon_0$, then surface impedance has the following simple form $\eta_s = 1/\sqrt{\epsilon_m}$ (CGI units) for any polarization and incidence angle of the incoming wave. In the case of finite-size structures, such as sequence of grooves shown in Figure 5.1 (a), in order for the impedance boundary condition to be valid at the interfaces with a filler dielectric, one has to demand that inside the notches only waves outgoing from the interfaces (into the notches) are excited, while no reflections from other surfaces reach those interfaces. Physically, this requires that waves propagating within the notches are either absorbed within the notch length, or that they are efficiently scattered within a notch and into the semi-infinite zone III, or that their coherence is somehow destroyed over the propagation distance within the notches via structured absorption of destructive interference as illustrated in Figure 5.1 (b)-(e). Note that when treating spoof plasmon waves on corrugated metallic surfaces, validity of IBC is easy to ascertain as long as the notch width is much larger than the metal skin depth. In this case, a wave transmitted into metal from the filler dielectric will decay exponentially fast from the interface into the notch and will have no presence at other surfaces. In contrast, in the case of spoof surface waves propagating on corrugated surfaces of lossless dielectrics, for IBC to be valid, it is not sufficient to demand that $\epsilon_m \gg \epsilon_0$, in addition, one has to ensure that experimental system includes one of the energy dissipation mechanisms described earlier that would prevent interaction between different interfaces of the same notch.

We now present brief derivation of the dispersion relation of spoof surface waves propagating on corrugated interfaces of dielectrics. First, we start with zone I that defines a planar waveguide filled with low permittivity ϵ_0 material, and that supports modes propagating along OZ direction. The modes are confined between the walls of high permittivity ϵ_m material. One end of the waveguide is opened into zone II, while the other one is bound by a high permittivity material. Assuming validity of the impedance boundary conditions, one can solve the Maxwell equations and find

dispersion relation of the groove waveguide even modes described by the propagation constant β_z^I that satisfies:

$$k_x^I \tan(k_x^I a/2) = -i \frac{k_0 \varepsilon_0}{\sqrt{\varepsilon_m}} \quad (5.2)$$

with $\beta_z^I = \pm \sqrt{\varepsilon_0 k_0^2 - (k_x^I)^2}$, where for a forward propagating wave (along OZ axis) $\text{Re}(\beta_z^I) > 0$, $\text{Im}(\beta_z^I) > 0$. Then, adapting an approach from the theory of spoof plasmons [51], in the limit of $dk_0 \sqrt{\varepsilon_0} \ll 1$ (subwavelength corrugation), an analytic expression for the propagation constant β_x^{SW} of a spoof surface wave propagating on the corrugated interface along the OX axis can be found by solving Maxwell equations in the zone II, while matching the fields with those of zone I and respecting the IBC along $z = 0$ on the notch surfaces:

$$\left(\frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} + k_z^{SW,II} \right) \frac{\sin(\beta_x^{SW} \frac{d}{2})}{\sin(\beta_x^{SW} \frac{a}{2})} = i \beta_z^I \frac{\sqrt{\varepsilon_m} \beta_z^I \tan(\beta_z^I h) + i \varepsilon_0 k_0}{\sqrt{\varepsilon_m} \beta_z^I - i \varepsilon_0 k_0 \tan(\beta_z^I h)} + \frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} \quad (5.3)$$

where $k_z^{SW,II} = \pm \sqrt{\varepsilon_0 k_0^2 - (\beta_x^{SW})^2}$ is the transverse (z-component) of the wave vector of a spoof surface wave in the filler dielectric (zone II), while $k_z^{SW,III} = \pm \sqrt{\varepsilon_m k_0^2 - (\beta_x^{SW})^2}$ is the transverse (z-component) of the wave vector of a spoof surface wave in the high permittivity dielectric (zone III) (see more details of derivation in the Supplemental Materials section). Although the derivations presented above assume a non-conductive material with purely real and positive value of ε_m , they also remain valid in case of lossy materials as long as $|\varepsilon_m| \gg \varepsilon_0$. Numerical methods such as the Newton-Raphson iteration method can then be used to solve Equations 5.2 and 5.3 together. In addition, in the most general case, the two dispersion relations 5.2 and 5.3 are universal functions of several non-dimensional variables namely $hk_0 \sqrt{\varepsilon_0}$, $ak_0 \sqrt{\varepsilon_0}$, $dk_0 \sqrt{\varepsilon_0}$, and $\sqrt{\varepsilon_0}/\sqrt{\varepsilon_m}$. Indeed, defining spoof surface wave effective refractive index as $n_{eff}^{SW} = \beta_x^{SW}/k_0$ and that of a groove waveguide as $n_{eff}^I = \beta_z^I/k_0$, as follows from the explicit forms of Equations 5.2 and 5.3:

$$\frac{n_{eff}^I}{\sqrt{\varepsilon_0}} = f_{n_{eff}^I} \left(ak_0 \sqrt{\varepsilon_0}, \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} \right) \quad (5.4)$$

$$\frac{n_{eff}^{SW}}{\sqrt{\varepsilon_0}} \simeq f_{n_{eff}^{SW}} \left(hk_0 \sqrt{\varepsilon_0}, ak_0 \sqrt{\varepsilon_0}, dk_0 \sqrt{\varepsilon_0}, \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} \right) \quad (5.5)$$

We will use Equations 5.4 and 5.5 later in the paper to evaluate the effects of geometrical and material parameters of the structured interface on the spoof surface wave dispersion relation. We

note that in addition to relations 5.2 and 5.3, dispersion relation of a spoof surface wave must satisfy several physical conditions:

$$\text{Re}(\beta_x^{SW}) > 0, \text{Im}(\beta_x^{SW}) > 0 \quad (5.6)$$

as all the materials in the system have real and positive values of the dielectric constants and no coherent back reflection is expected for corrugation with a deeply subwavelength period. At the same time, a properly defined physical solution requires that electromagnetic energy be localized near the corrugated surface while decaying away from the interface in both zone II and zone III. Thus, the signs of $k_z^{SW,II}$ and $k_z^{SW,III}$ in Equations 5.2 and 5.3 must be chosen so that:

$$\text{Im}(k_z^{SW,II}) > 0, \text{Im}(k_z^{SW,III}) < 0 \quad (5.7)$$

One generally finds that in case of a forward travelling spoof surface wave with dispersion relation respecting Equations 5.6 and 5.7, and similarly to the case of a classic Brewster wave [137], the wave phase front in zone II is traveling toward the interface, while in zone III it travels away from the interface:

$$\text{Re}(k_z^{SW,II}) < 0, \text{Re}(k_z^{SW,III}) < 0 \quad (5.8)$$

This is also the reason why Brewster waves are closely related to the phenomenon of a Brewster angle [147]. Also, modal propagation distance L_x , as well as modal extent into the filler dielectric L_z^{II} can be defined as distances over which the fields decay by a factor e in the corresponding directions (+X, +Z):

$$L_x = 1/|\text{Im}(\beta_x^{SW})| \quad (5.9)$$

$$L_z^{II} = 1/|\text{Im}(k_z^{SW,II})| \quad (5.10)$$

We note that for a spoof surface wave to be properly defined one must require that its transverse sizes be much smaller than the propagation distance $L_z^{II} \ll L_x$.

5.4.1 Case of infinite positive permittivity $\epsilon_m = +\infty$

In this section, a case of a corrugated structure made of a perfect isolator ($\epsilon_m = +\infty$) will be considered in order to find the spoof surface wave cut-off frequencies and its dispersion in this simple limit. By considering $\epsilon_m = +\infty$ one can greatly simplify the analytic dispersion relations 5.2 and 5.3 as follow:

$$\beta_z^l = \pm \sqrt{\varepsilon_0 k_0^2 - \left(\frac{2\pi}{a} l\right)^2}, \quad l = 0, 1, 2, \dots \quad (5.11)$$

$$k_z^{SW, II} \frac{\sin(\beta_x^{SW} \frac{d}{2})}{\sin(\beta_x^{SW} \frac{a}{2})} = i \beta_z^l \tan(\beta_z^l h) \quad (5.12)$$

These expressions allow to find frequency regions of spoof surface wave existence. Thus, a new branch of the spoof surface wave dispersion relation will be pulled from the radiation continuum (lower cut-off frequency) when $k_z^{SW, II} = 0 \rightarrow \beta_z^l h = \pi \cdot l_c$, while the same branch will be terminated at higher frequencies (upper cut-off frequency) when spoof surface wave propagation constant becomes infinite when $\tan(\beta_z^l h) = \infty \rightarrow \beta_z^l h = \pi/2 + \pi \cdot l_c$. From Equation 5.11 we then find the following expression for the frequency regions of existence of the spoof surface waves:

$$\nu_c \in \frac{c}{\sqrt{\varepsilon_0}} \left(\sqrt{\left(\frac{l}{a}\right)^2 + \left(\frac{l_c}{2h}\right)^2}, \sqrt{\left(\frac{l}{a}\right)^2 + \left(\frac{l_c+0.5}{2h}\right)^2} \right); \quad l = 0, 1, 2, \dots, \quad l_c = 0, 1, 2, \dots \quad (5.13)$$

while for the fundamental branch ($l = 0; l_c = 0$) it translates into $\nu_c \in (0, c/(4h\sqrt{\varepsilon_0}))$.

Expression 5.12 can be further simplified in the regime of subwavelength corrugation $|\beta_x^{SW}|d \ll 1$, there spoof surface wave dispersion relation and its penetration depth into the filler dielectric L_z^{II} can be written as:

$$\beta_x^{SW} = \sqrt{\varepsilon_0 k_0^2 + \left[\beta_z^l \tan(\beta_z^l h) \left(\frac{a}{d}\right) \right]^2}; \quad \varepsilon_{eff}^{SW} \simeq \varepsilon_0 + \left[\frac{a}{d} \frac{\beta_z^l}{k_0} \tan(\beta_z^l h) \right]^2 \quad (5.14)$$

$$L_z^{II} = \frac{1}{\beta_z^l \tan(\beta_z^l h) \left(\frac{a}{d}\right)} \quad (5.15)$$

From these expressions it follows that the spoof surface wave confinement in the filler dielectric can become subwavelength $L_z^{II} k_0 < 1$ when certain conditions on the groove depth are satisfied. Thus, for the fundamental mode of a groove $\beta_z^l = \sqrt{\varepsilon_0} k_0$, condition of subwavelength confinement at the surface vicinity in the filler dielectric becomes:

$$\tan(\sqrt{\varepsilon_0} k_0 h) > \left(\frac{d}{a}\right) \frac{1}{\sqrt{\varepsilon_0}} \quad (5.16)$$

signifying that subwavelength confinement is observed mostly in the vicinity of an upper cut-off frequency. In Figure 5.2 (a) (red dashed curve) we present a typical dispersion relation of a spoof

surface wave using analytical dispersion relation 5.14 for $d = 1.5a$ while assuming that a subwavelength corrugation $|\beta_x^{SW}|d \ll 1$ holds for all the parameters and all frequencies. A subwavelength corrugation period $d = 45 \text{ } \mu\text{m} < \lambda_0/5$ along with the depth of the grooves $h = 75 \text{ } \mu\text{m}$ are chosen so that the upper cut-off frequency of the fundamental branch is at $\nu_c = 1 \text{ THz}$ ($\lambda_0 = 300 \text{ } \mu\text{m}$), while we suppose that filler dielectric is air $\epsilon_0 = 1$. In black curve we present numerical solution of Equations 5.11 and 5.12 solved with the Newton-Raphson iteration method for the same structure. The gray region represents the regime where the subwavelength corrugation condition does not hold. The spoof surface wave penetration depths L_z^H/λ into the filler dielectric as calculated using the dispersion relation in the long wavelength limit 5.14 (solid curve), and numerically solved one 5.12 (dashed curve) are presented in Figure 5.2 (b). The subwavelength localization of the spoof surface wave near the interface is possible near the upper cut-off frequency. Finally, we note that when approaching the upper cut-off frequency, solution of Equations 5.11 and 5.12 might also give high values of the spoof surface wave propagation constant $|\beta_x^{SW}|d \gtrsim 1$, which eventually results in breaking down of the long wavelength approximation that was used to derive Equations 5.3 and 5.12. Thus, both expressions 5.12 and 5.14 are expected to give invalid solutions in the gray area. Otherwise, while respecting the subwavelength regime condition, both dispersion relation 5.12 and 5.14 are similar, and so the simplified analytical could be effectively used to represent the dispersion relation of spoof surface wave where $\epsilon_m \rightarrow \infty$. Also, we note that when tighter confinement of a Spoof wave near surface is desired, one must resort to smaller periods d , that will allow operation closer to the upper cut-off frequency.

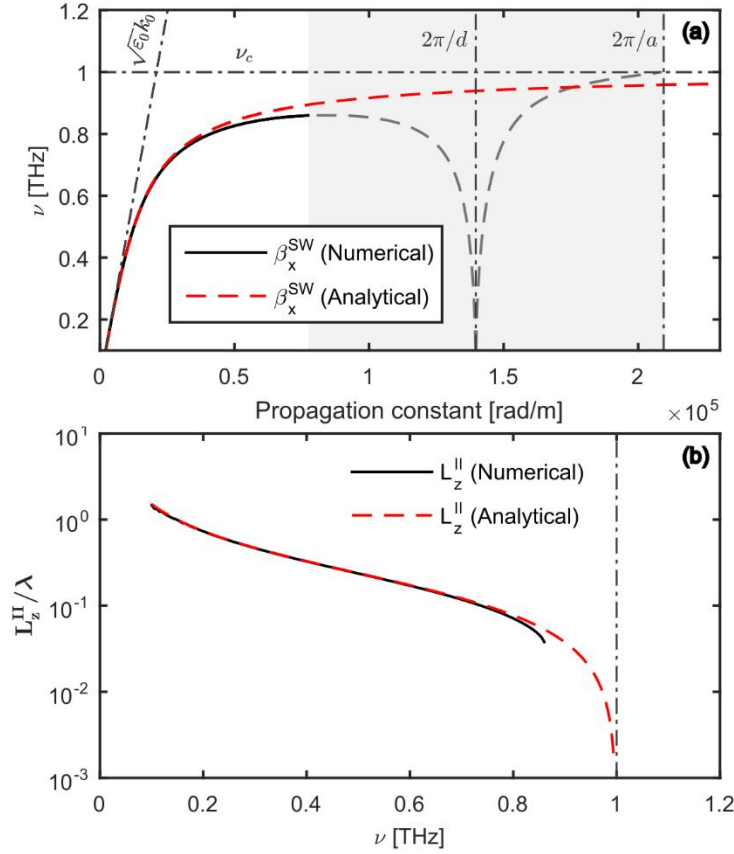


Figure 5.2 Dispersion relation of a spoof surface wave for the case of perfect isolator $\epsilon_m = +\infty$. (a) Dispersion relation of a spoof surface wave using analytical approximation 5.14 (dashed red) and by numerically solving Equation 5.12 (solid black) with the Newton-Raphson iteration method. (b) Penetration depth of the spoof surface wave into filler dielectric (Zone II) as defined by the analytical expression 5.15 (dashed red) and from numerical solution 5.12 (solid black) in the units of a free space wavelength λ . Here, $d = 45 \mu\text{m}$, $a = 30 \mu\text{m}$ and $h = 75 \mu\text{m}$.

5.4.2 Case of finite positive permittivity ϵ_m

Governing equations for the dispersion relation of a spoof surface wave with finite permittivity ϵ_m as given by Equations 5.2 and 5.3 can be simplified in various limits. First of all, we note that in case of subwavelength corrugation $dk_0 \ll 1$, Equation 5.2 can be solved analytically via linearization as $|k_x^l| a/2 \ll 1$ for any choice of a , and k_0 (indeed, linearization of Equation 5.2 only requires that $ak_0 \ll 2\sqrt{\epsilon_m}/\sqrt{\epsilon_0}$). Furthermore, assuming a long wavelength limit $|\beta_x^{sw}|d \ll$

1 we get an analytic expression for the effective permittivity of a lossy fundamental spoof surface wave:

$$\beta_z^I = \sqrt{\varepsilon_0 k_0^2 + i \frac{2k_0 \varepsilon_0}{a\sqrt{\varepsilon_m}}} \quad (5.17)$$

$$\varepsilon_{eff}^{SW} \simeq \varepsilon_0 - \left[\frac{a \beta_z^I \varepsilon_0 k_0 - i \sqrt{\varepsilon_m} \beta_z^I \tan(\beta_z^I h)}{d k_0 \sqrt{\varepsilon_m} \beta_z^I - i \varepsilon_0 k_0 \tan(\beta_z^I h)} + \frac{\varepsilon_0}{\sqrt{\varepsilon_m}} \left(\frac{d-a}{d} \right) \right]^2 \quad (5.18)$$

Note that in this regime, the two dispersion relations are only functions of a few non-dimensional parameters namely $hk_0\sqrt{\varepsilon_0}$, a/d , $\sqrt{\varepsilon_0}/\sqrt{\varepsilon_m}$, and $1/ak_0\sqrt{\varepsilon_m}$ such as:

$$\frac{n_{eff}^I}{\sqrt{\varepsilon_0}} = f_{n_{eff}^I} \left(\frac{1}{ak_0\sqrt{\varepsilon_m}} \right) \quad (5.19)$$

$$\frac{n_{eff}^{SW}}{\sqrt{\varepsilon_0}} \simeq f_{n_{eff}^{SW}} \left(hk_0\sqrt{\varepsilon_0}, \frac{a}{d}, \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}}, \frac{1}{ak_0\sqrt{\varepsilon_m}} \right) \quad (5.20)$$

Understanding validity condition $|\beta_x^{SW}|d \ll 1$ for Equation 5.18 is somewhat complicated as in the vicinity of the upper cut-off frequency $\beta_z^I h \sim \pi/2$, the values of $\tan(\beta_z^I h)$ become large and the spoof surface wave effective refractive index can also becomes large ($n_{eff}^{SW} \sim \sqrt{\varepsilon_m}$) both in its real and imaginary parts. Thus, for relation 5.18 to be valid for any choice of parameters, a , d , h in the vicinity of a cut-off frequency $\beta_z^I h \sim \pi/2$, one must require that $ak_0 \ll 1/\sqrt{\varepsilon_m}$. This requirement of extremely subwavelength grooves can lead to significant losses of spoof surface waves due to inefficient confinement, and as a consequence, high radiation losses in such grooves as follows from Equation 5.17. In practice, in order to minimize radiation loss in the grooves one would rather choose $ak_0 \gg 1/\sqrt{\varepsilon_m}$, therefore Equation 5.18 is not expected to be valid in the immediate vicinity of the upper cut-off frequency $\beta_z^I h \sim \pi/2$, while it will be generally valid somewhat away from the cut-off frequency. Thus, assuming $ak_0 \gg 1/\sqrt{\varepsilon_m}$ and $\frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m} \ll \tan(hk_0\sqrt{\varepsilon_0})} \ll \sqrt{\varepsilon_m}/\sqrt{\varepsilon_0}$, Equations 5.17 and 5.18 can be further simplified to give:

$$\beta_z^I \simeq \sqrt{\varepsilon_0} k_0 + i \frac{\sqrt{\varepsilon_0}}{a\sqrt{\varepsilon_m}} \quad (5.21)$$

$$\varepsilon_{eff}^{SW} \simeq \varepsilon_0 + \left[\frac{a \beta_z^I}{d k_0} \tan(\beta_z^I h) \right]^2 \quad (5.22)$$

Furthermore, in the case of a relatively shallow corrugation $\sqrt{\varepsilon_0}/\sqrt{\varepsilon_m} \ll \sqrt{\varepsilon_0}k_0h \ll 1$, this can be further simplified to give a relatively simple expression for the spoof surface wave refractive index. It can be also verified that in this limit spoof surface wave is well defined in a sense that its penetration depth into zone II is much smaller than its propagation length:

$$\beta_z^I \simeq \sqrt{\varepsilon_0}k_0 + i \frac{\sqrt{\varepsilon_0}}{a\sqrt{\varepsilon_m}} \quad (5.23)$$

5.4.3 Spatial localization and propagation distance of spoof surface waves

In Figure 5.3 we study in more details the choice of design parameters and their effect on the propagation distance and localization of spoof surface waves in the semi-infinite cladding region (zone II). Our main question is whether spoof surface waves are well defined. We consider that a surface wave is well defined when its propagation distance is much larger than the wave extent into a lower permittivity cladding $L_z^{II} < L_x$ as defined in Equations 5.9 and 5.10. In this study, we resort to numerical solution of the full formulations 5.2 and 5.3 for dispersion relation of the fundamental spoof surface wave. Particularly, from analysis of Equations 5.17-5.20 derived under assumption of subwavelength corrugation ($\beta_x^{SW}d \ll 1$) it follows that a critical design parameter defining spoof surface wave loss is $1/ak_0\sqrt{\varepsilon_m}$ as it also defines radiation losses of a single groove waveguide. Next, without the loss of generality we fix $d = 1.5a$ and $\nu = 1\text{Hz}$, and assume that the filler dielectric is air $\varepsilon_0 = 1$. We then study dependence of the normalized spoof surface propagation distance $L_xk_0/\sqrt{\varepsilon_0}$, as well as the wave penetration into the filler material $L_z^{II}k_0/\sqrt{\varepsilon_0}$ as a universal function of the corrugation depth parameter $hk_0\sqrt{\varepsilon_0}$ and the groove waveguide loss parameter $1/ak_0\sqrt{\varepsilon_m}$ (see Figure 5.3). Note that in the limit of low losses $1/ak_0\sqrt{\varepsilon_m} \ll 1$, we expect the maximal confinement near the upper cut-off frequency defined by $hk_0\sqrt{\varepsilon_0} = \pi/2$. We also present results for several values of the high permittivity dielectric $\varepsilon_m = 100, 1000, \text{ and } 10000$. Additionally, in Figure 5.3 in gray we identify the regions where subwavelength corrugation condition $\beta_x^{SW}d < 1$ does not hold, and, therefore, the found dependencies are not universal (or might have limited validity) when using the nondimensional parameters $1/ak_0\sqrt{\varepsilon_m}$, $hk_0\sqrt{\varepsilon_0}$ (for fixed values of a/d and $\varepsilon_0/\varepsilon_m$) as predicted by Equations 5.19 and 5.20. Black regions in Figure 5.3 define parameter space where either numerical solution is not found or physical conditions 5.6 and 5.7 for the existence of a forward propagating spoof surface wave are not respected. Finally,

dashed curves in Figure 5.3 border the regions where the modal confinement in the filler dielectric becomes subwavelength $L_z^H = \lambda/\sqrt{\epsilon_0}$ or where the spoof surface wave becomes well defined $L_z^H/L_x = 1$. Thus, a design parameter space that would, for example, result in a well-defined spoof surface wave with subwavelength extent into the filler dielectric will be between the two dashed lines shown in Figure 5.3 (see second and third row of panels).

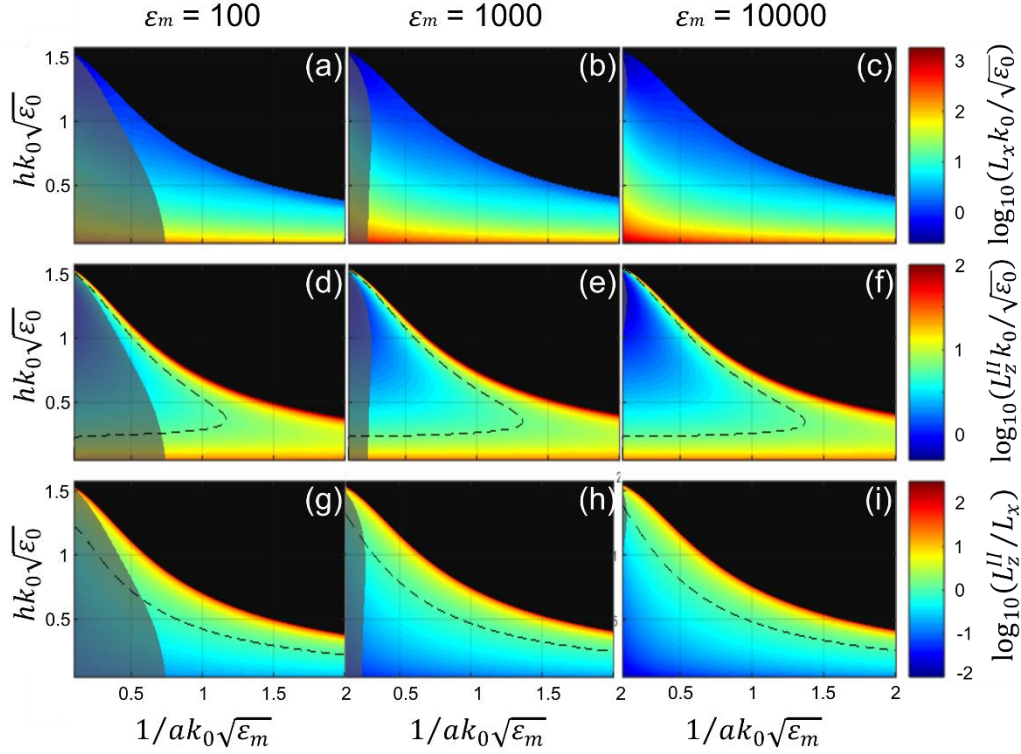


Figure 5.3 Various properties and regimes of spoof surface wave supported by the corrugated structure. (a)-(c) Normalized propagation distance $L_x k_0 / \sqrt{\epsilon_0}$, (d)-(f) Normalized penetration into the filler dielectric material $L_z^H k_0 / \sqrt{\epsilon_0}$, (g)-(i) the ratio between the penetration into the filler dielectric material L_z^H and the propagation distance L_x are presented in function of the parameters $1/ak_0\sqrt{\epsilon_m}$ and $hk_0\sqrt{\epsilon_0}$ for respectively $\epsilon_m = 100$, $\epsilon_m = 1000$, and $\epsilon_m = 10000$. The regions in gray indicate non-subwavelength regime. The dashed lines indicate (d)-(f) the subwavelength limit $L_z^H k_0 \sqrt{\epsilon_0} = 2\pi$ and (g)-(i) the well-defined surface wave limit $L_z^H/L_x = 1$. Here, the operational frequency is 1 THz and $d = 1.5a$.

From the presented data we conclude that subwavelength confinement of a spoof surface wave can be achieved near the upper cut-off frequency (larger values of $hk_0\sqrt{\varepsilon_0}$ bordering black regions in Figure 5.3), when minimizing the radiation losses of a groove waveguide (smaller values of $1/ak_0\sqrt{\varepsilon_m}$). At the same time, in this region of design space propagation distance L_x can become smaller than the modal transverse size L_z^H , thus rendering spoof waves ill-defined. However, by somewhat reducing the groove depth $hk_0\sqrt{\varepsilon_0}$ (while still operating outside of the gray region) allows the propagation distance L_x to increase while retaining strong modal confinement near the interface. Finally, increasing the permittivity ε_m , allows to reduce the propagation loss of a spoof surface mode, extend its propagation distance L_x , as well as to increase the validity region of the subwavelength corrugation condition $\beta_x^{SW}d < 1$ (resulting in smaller gray areas in Figure 5.3). Validity of the subwavelength corrugation condition can be also extended by choosing a deeply subwavelength period d .

5.5 Physical meaning of the spoof waves on non-conductive interfaces

In the previous sections, a dispersion relation for the spoof surface wave propagating along a corrugated non-conductive interface was derived and studied by using field expansions in terms of planewaves in various regions of a structure, while enforcing the field continuity and boundary conditions. While mathematically sound, the physical meaning of the surface waves was somewhat obscured. To demystify the nature of surface waves on the corrugated non-conductive interfaces, a simple effective medium model for the interfacial layer can be used. Particularly, assuming optically thin features of the surface corrugation $a\varepsilon_0 \ll \lambda, (d-a)\varepsilon_m \ll \lambda$, as well as a period which is much smaller than the corrugation height $d \ll h$, the corrugated interface can be approximated as a uniform anisotropic layer of thickness h . The effective permittivity of the corrugated layer can be described using a diagonal tensor $(\varepsilon_c^x, \varepsilon_c^y, \varepsilon_c^z)$, where:

$$\varepsilon_c^x = d \left(\frac{a}{\varepsilon_0} + \frac{d-a}{\varepsilon_m} \right)^{-1} \quad (5.24)$$

$$\varepsilon_c^y = \varepsilon_c^z = \frac{a}{d} \varepsilon_0 + \frac{d-a}{d} \varepsilon_m \quad (5.25)$$

The interfacial layer is sandwiched between two homogeneous isotropic non-conductive materials with $\varepsilon_0 > 0$, $\varepsilon_m > 0$, while the permittivity constants satisfy $\varepsilon_0 < \varepsilon_c^z < \varepsilon_c^y = \varepsilon_c^z < \varepsilon_m$ as

illustrated in Figure. 5.4. As we will show in the following, the interfacial layer supports a leaky mode that is guided along the interface, while showing evanescent decay into the top cladding and radiation leakage into the bottom cladding. This guided leaky mode is the spoof surface mode analogous to what is described in the previous sections.

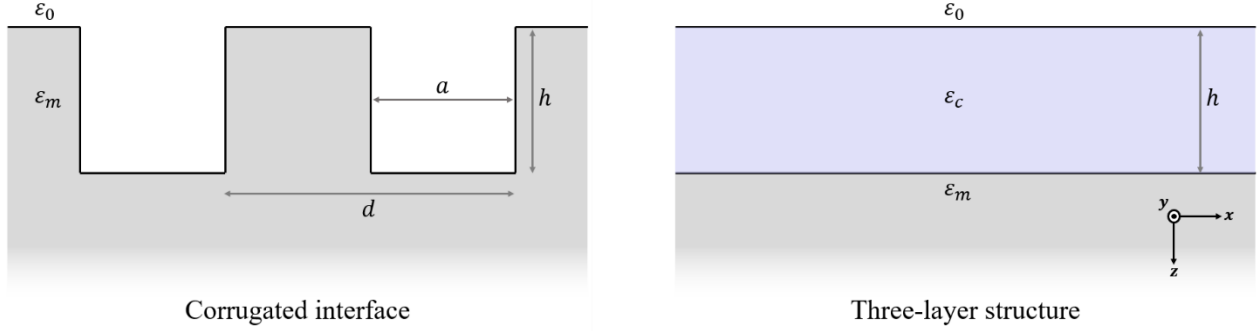


Figure 5.4 A corrugated interface between two con-conductive materials can be analysed as a three-layer structure with the middle layer being a uniform anisotropic material with electric permittivity described by a diagonal tensor.

Indeed, following [148], guided mode supported by the anisotropic interfacial layer can be found using a Transfer Matrix theory. Particularly, assuming only outgoing planewaves $B \cdot \exp(i\beta x - ik_0^z z)$ in the top cladding, and $A \cdot \exp(i\beta x + ik_m^z z)$ in the bottom claddings, where:

$$k_{0,m}^z = \sqrt{\varepsilon_{0,m} k_0^2 - \beta^2} \quad (5.26)$$

then, the amplitudes of the two outgoing waves are related by a 2x2 transfer matrix T (see Supplementary materials for more details):

$$\begin{bmatrix} A \\ 0 \end{bmatrix} = T \begin{bmatrix} 0 \\ B \end{bmatrix} \quad (5.27)$$

Solving Equation 5.27 allows to find a complex dispersion relation of the interfacial leaky mode as detailed in Supplementary materials. In particular, for the case of $\varepsilon_m \rightarrow \infty$ we find that $\varepsilon_c^x \approx d/(a\varepsilon_0)$, $\varepsilon_c^y = \varepsilon_c^z \approx (d-a)/(d\varepsilon_m) \rightarrow \infty$, $k_c^z \approx \sqrt{\varepsilon_c^x} k_0$, which allows one to find dispersion relation of the guided mode in a simple analytical form:

$$\varepsilon_{eff}^{SW} = \frac{\beta^2}{k_0^2} \simeq \varepsilon_0 \left(1 + \frac{a}{d} \tan^2 \left(\sqrt{\frac{d}{a}} \varepsilon_0 k_0 h \right) \right) \quad (5.28)$$

Interestingly, the obtained dispersion relation (Equation 5.28) is somewhat different from the one found earlier (Equation 5.14). The difference stems from different approximations made in the derivation of these dispersion relations. Particularly, in order to approximate the corrugated layer as a uniform anisotropic dielectric it is important that all the corrugation features are optically thin $a \ll \lambda/\varepsilon_0$, $(d - a) \ll \lambda/\varepsilon_m$. Thus, in the case of a perfect isolator $\varepsilon_m \rightarrow \infty$, its thickness in the corrugation has to be vanishingly small $(d - a) \rightarrow 0$. This is in contract with the assumptions made in the previous sections when deriving dispersion relation (Equation 5.14). There, we only assume a subwavelength corrugation period $d \ll \lambda/\varepsilon_0$, while we put no limitation on the optical thickness of a perfect isolator. Instead, we assume that whatever radiation enters the perfect isolator layer, it is incoherently scattered or absorbed within the isolator.

5.6 Comparison of analytical and numerical results using IBC

In this section, we study in more detail dispersion relation of spoof surface waves on corrugated surfaces as a function of its various parameters. Studied geometry is presented in Figure 5.1 (a), with all the boundaries between the filler dielectric and the high dielectric constant material being of the IBC type. The results of semi-analytical calculations 5.2 and 5.3 are verified using finite element COMSOL mode solver with Floquet boundary conditions along the modal propagation direction (see more details in Supplementary Materials). The Figure 5.5 compares dispersion relations of the fundamental spoof surface wave supported by the corrugated surface made of materials with purely real and positive permittivity as obtained by solving Equations 5.2 and 5.3 using the Newton-Raphson iteration method (solid), with that computed using COMSOL solver (dashed). Here, we use $d = 50 \mu\text{m}$, $a = 35 \mu\text{m}$ and $h = 75 \mu\text{m}$, and frequencies in the (0.1-1 THz) range. For the materials, we use $\varepsilon_0 = 1$ and $\varepsilon_m = 100$, which corresponds respectively to the relative dielectric permittivity of air and TiO_2 [149]. The upper cut-off frequency for the fundamental spoof surface mode is given by Equation 5.13 where $l_c = 0, l = 0$, and it equals to 0.95 THz. Real and imaginary parts of the corresponding dispersion relation are shown in Figure 5.5 (a), while the corresponding modal propagation distance and transverse size are shown in Figure 5.5 (b). We note that near the upper cut-off frequency, modal transverse size decreases dramatically and quickly becomes subwavelength (see Figure 5.5 (c)). However, when operating too close to the upper cut-off frequency, there is a significant increase in the radiation loss into zone III, thus leading to much shorter propagation distances. As seen from Figure 5.5, there exists

an optimal spectral region where transverse modal confinement is subwavelength, while propagation distance is larger than the wave transverse size.

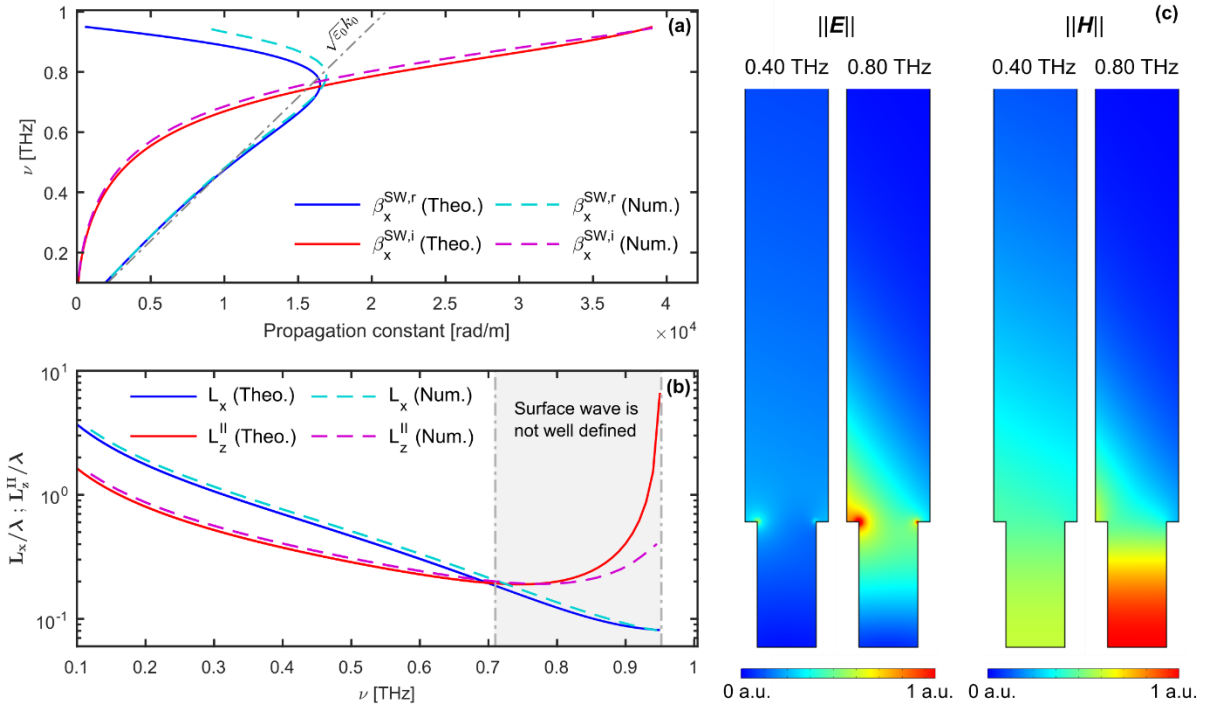


Figure 5.5 Typical dispersion relation of spoof surface wave supported by the corrugated surface. (a) Complex dispersion relation of a fundamental spoof surface wave as found by solving Equations 5.2 and 5.3 using Newton-Raphson iteration method (solid curves) are compared to those found by COMSOL (dashed curves). (b) Propagation distance L_x (blue, cyan) and penetration depth into air L_z^{II} (red, magenta) in units of λ . (c) Distribution of the electric and magnetic field amplitudes in air at 0.40 THz and 0.80 THz found using COMSOL. Here, $d = 50 \mu\text{m}$, $a = 35 \mu\text{m}$, $h = 75 \mu\text{m}$, $\epsilon_0 = 1$ and $\epsilon_m = 100$.

Next, we study the effects of the groove width to period ratio a/d , and groove height h on the spoof surface wave dispersion, as well as validity of the semi-analytical formulations 5.2 and 5.3 when describing such waves. In Figure 5.6 we present modal dispersion relation when varying groove width a for a fixed period $d = 50 \mu\text{m}$ and groove height $h = 75 \mu\text{m}$. From these results, we observe that increasing groove width a somewhat increases the upper cut-off frequency of the fundamental spoof surface wave, while it significantly increases the modal losses. For high enough values of a , dispersion relation of a spoof surface wave crosses the light line of the filler dielectric

and extends further toward higher values of the propagation constant, which leads to stronger modal confinement at the interface. One way to understand this phenomenon is to note that larger groove sizes lead to stronger modal presence in the grooves, as well as stronger radiation losses at the bottom of the planar waveguides (zone I) that radiate into zone III through their openings of size a .

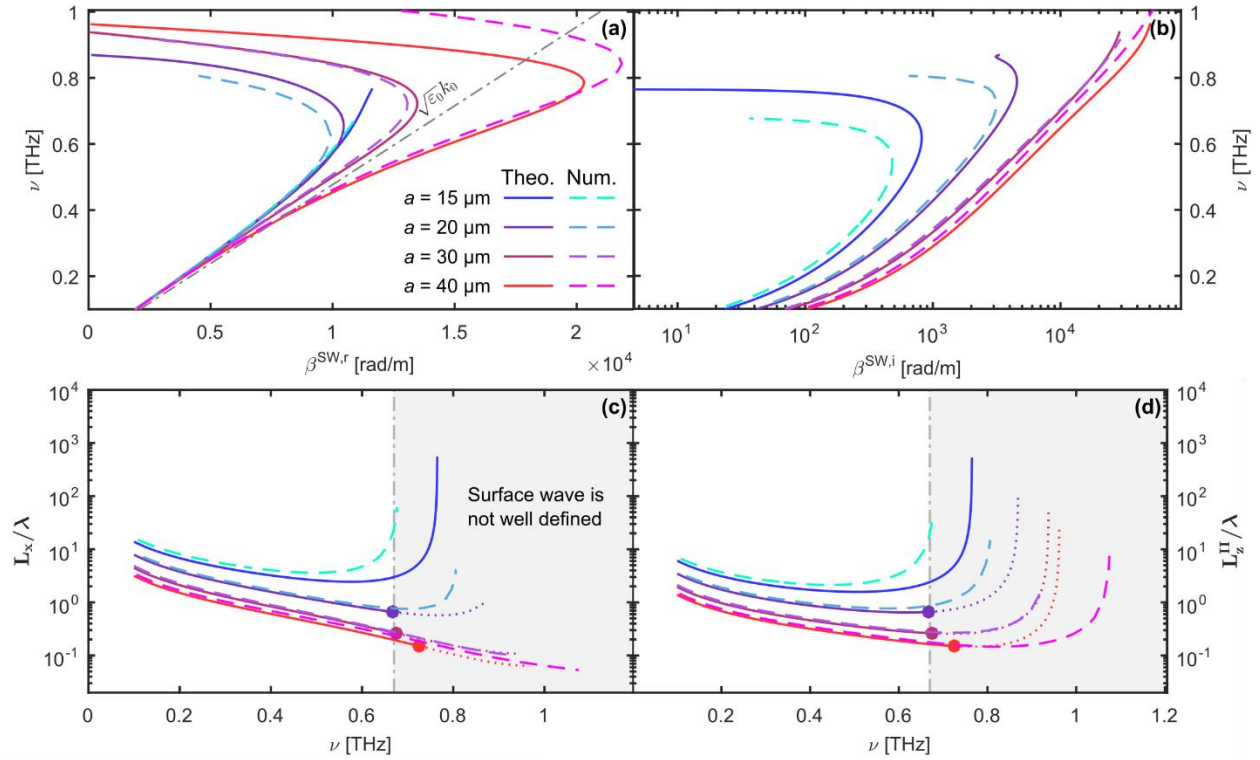


Figure 5.6 Propagation constant of spoof surface wave for various groove width a . (a) Real part and (b) imaginary part of the propagation constant of the fundamental spoof surface wave for three structures of increasing groove width $a = 15 \mu\text{m}$, $20 \mu\text{m}$, $30 \mu\text{m}$, and $40 \mu\text{m}$. (c) Propagation distance L_x and (d) penetration depth into air L_z^{II} in units of λ . Results are found by solving Equations 5.2 and 5.3 using Newton-Raphson iteration method (solid curves) are compared to those found by COMSOL (dashed curves). The circles presented in (c) and (d) indicate the limit where the surface wave is well-defined $L_x/L_z^{\text{II}} = 1$. The period d is $50 \mu\text{m}$, the groove depth h is $75 \mu\text{m}$ and the permittivity constants are $\epsilon_0 = 1$ and $\epsilon_m = 100$.

Finally, in Figure 5.7, we study the effect of the groove height on the modal dispersion relation, where $d = 50 \mu\text{m}$, and $a = 25 \mu\text{m}$. Here, as expected, we observe that deeper grooves result in

lower cut-off frequencies, and higher propagation losses. To appreciate the effect of the groove height on the dispersion relation, in Figure 5.8 we also present the results at a fixed operational frequency 1 THz, and fixed period $d = 50 \mu\text{m}$ and groove width $a = 25 \mu\text{m}$, while varying the groove height h . From this data we see that choosing shallow grooves (small h) results in longer propagation distances of a spoof surface wave, as well as its stronger presence in the filler dielectric. Higher losses for deeper grooves are easy to understand by noting that radiation in a spoof surface wave is partially guided along the leaky waveguide (zone I), so longer waveguides naturally result in higher (almost exponentially with h) losses. By increasing the groove height one can, in principle, retain acceptable modal propagation distances, while also increasing modal confinement to within several wavelengths at the structured surface.

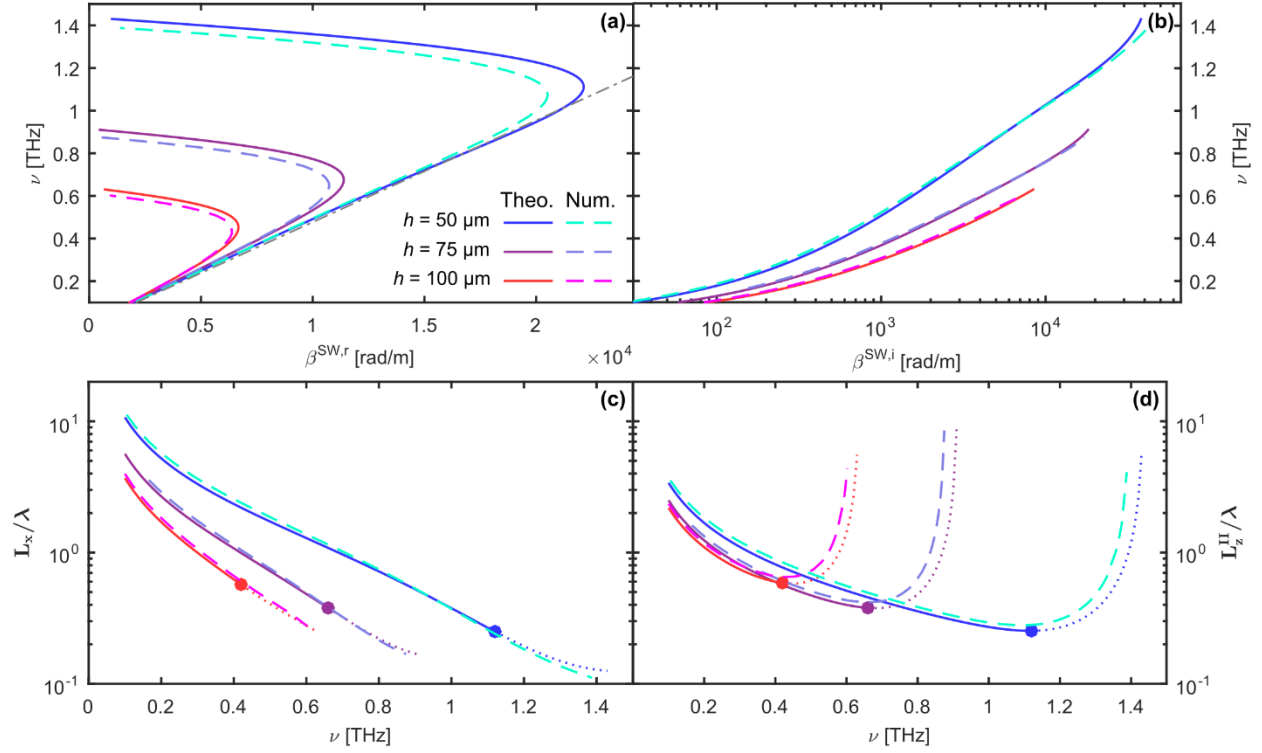


Figure 5.7 Propagation constant of spoof surface wave for various groove height h . (a) Real part and (b) imaginary part of the propagation constant of the fundamental spoof surface wave for three structures of increasing groove height $h = 50 \mu\text{m}$, $h = 75 \mu\text{m}$ and $h = 100 \mu\text{m}$. (c) Propagation distance L_x and (d) penetration depth into air L_z^{II} in units of λ . Results are found by solving Equations 5.2 and 5.3 using Newton-Raphson iteration method (solid curves) are compared to those found by COMSOL (dashed curves). The circles presented in (c) and (d) indicate the limit where the surface wave is well-defined $L_x/L_z^{\text{II}} = 1$. The period d is 50 μm , the groove width a is 25 μm and the permittivity constants are $\epsilon_0 = 1$ and $\epsilon_m = 100$.

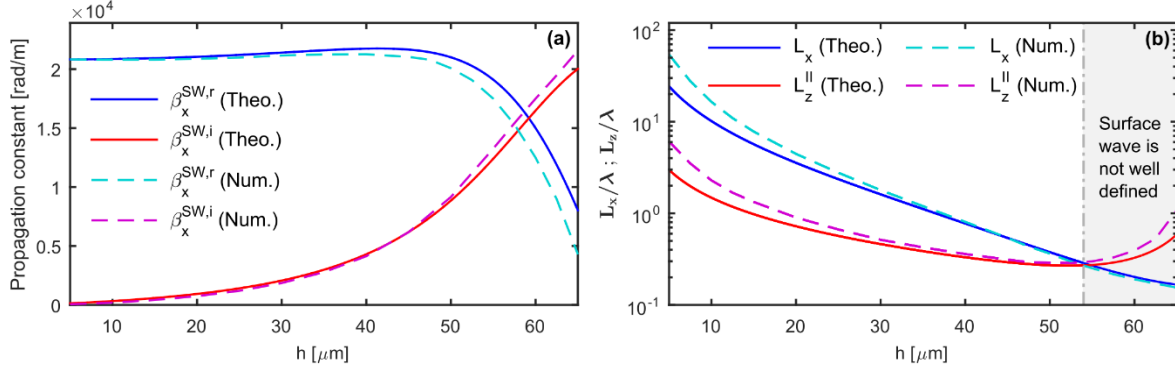


Figure 5.8 Propagation constant and modal sizes as a function of the groove depth h at 1 THz operation frequency. (a) Real and imaginary parts of the fundamental spoof surface wave propagation constant as a function of the groove depth. (b) Propagation distance L_x and penetration depth into air L_z^{II} in units of λ . Results are found by solving Equations 5.2 and 5.3 using Newton-Raphson iteration method (solid curves) are compared to those found by COMSOL (dashed curves). Here, $a = d/2$, $d = 50 \mu\text{m}$ and the permittivity constants are $\epsilon_0 = 1$ and $\epsilon_m = 100$.

5.7 Validity of the impedance boundary conditions and limitations

Up to now, the impedance boundary conditions have been used to demonstrate the possibility of propagation of spoof surface waves along corrugated structures made of non-conductive materials. Physically, IBC limits the field presence only to the low dielectric permittivity filler region, while neglecting the effects of field penetration into the high dielectric permittivity material. In reality, the electromagnetic fields localized at the corrugated interface can penetrate into structured high dielectric permittivity material and interfere within the notches. Despite the fact that electric field will be vanishingly small compared to the magnetic field in the limit $\epsilon_m \rightarrow +\infty$, this alone does not prevent coupling of the fields in adjacent grooves via non-zero magnetic field in the notches. Therefore, even in the limit of infinitely high ϵ_m , one still has to rely on one of the several decoherence mechanisms such as scattering, absorption or radiation within the notches (see Figure 5.1), so that the formulation using IBC remains valid. In practice, however, we often observe that numerical simulations of a complete system that includes high dielectric permittivity material indeed match those with IBC. This happens because interaction between adjacent notches is suppressed via a combination of destructive interferences of the electromagnetic fields inside the

notches, as well as strong radiation loss into the semi-infinite high permittivity dielectric from the narrow notches. For example, in Figure 5.9 we compare dispersion relations of spoof surface waves as computed using either a semi-analytical formulations 5.2 and 5.3 with IBC, or using COMSOL with all the zones I, II, and III explicitly present in simulations (zone III is terminated with the Perfectly Matched Layer absorbing boundary domain, for more information see Supplementary Materials).

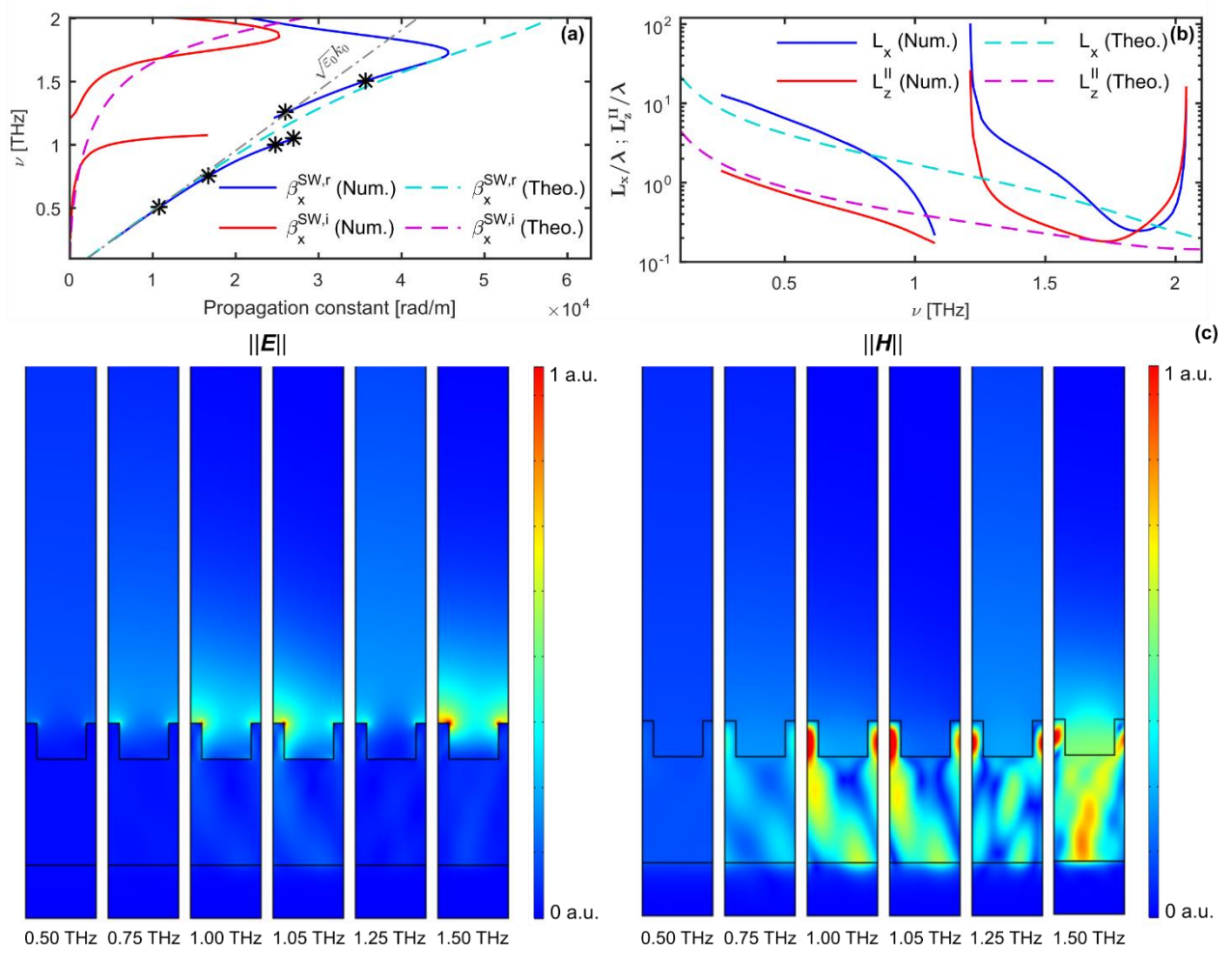


Figure 5.9 Dispersion relation of spoof surface waves computed using full geometry of the corrugated surface (zones I, II, and III, without IBC) terminated with a perfectly matched layer. (a) Real (blue, cyan) and imaginary (red, magenta) parts of the spoof surface wave propagation constant as found using COMSOL simulation of a complete geometry (solid), and as computed Equations 5.2 and 5.3 (dotted). (b) Propagation distance (blue, cyan) and penetration depth into air (red, magenta) in units of λ . (c) Distribution of the electric and magnetic fields at various frequencies 0.50 THz (no resonance in the notch), 0.75 THz, 1.00 THz (resonance in the notch), 1.05 THz, 1.25 THz, and 1.50 THz. Here, $d = 50 \mu\text{m}$, $a = 35 \mu\text{m}$, $h = 25 \mu\text{m}$, $\epsilon_0 = 1$ and $\epsilon_m = 100$.

As seen from the figure, at most frequencies there is a good comparison between the two dispersion relations with the exception of certain frequencies where a resonance is excited inside the notches

as seen in Figure 5.9 (c). We, therefore, conclude that our semi-analytical formulations 5.2 and 5.3 derived using IBC, can indeed describe dispersion relation of spoof surface waves propagating on non-conductive corrugated surfaces. This semi-analytical model, however, is limited when adjacent grooves are strongly coupled via resonant field excitation inside of the high permittivity notches. One way to ensure the validity of the IBC approximation is to use scattering or perfect absorber medium in the notches in order to avoid field coupling as discussed earlier. In practice, small irregularities in the periodicity of the corrugated structure, along with lossy material are also expected to reduce the field coupling through the notches. Thus, one can identify a limit in the validity of the IBC approximation for any operational frequency based on the absorption coefficient of the high-permittivity material. In Figure 5.10, the relation between the propagation constant and the imaginary part of the refractive index of the high permittivity material is illustrated for the same structure previously presented in Figure 5.9, along with an operational frequency of 1 THz, which corresponds to a resonant frequency in the case of the lossless structured surface.

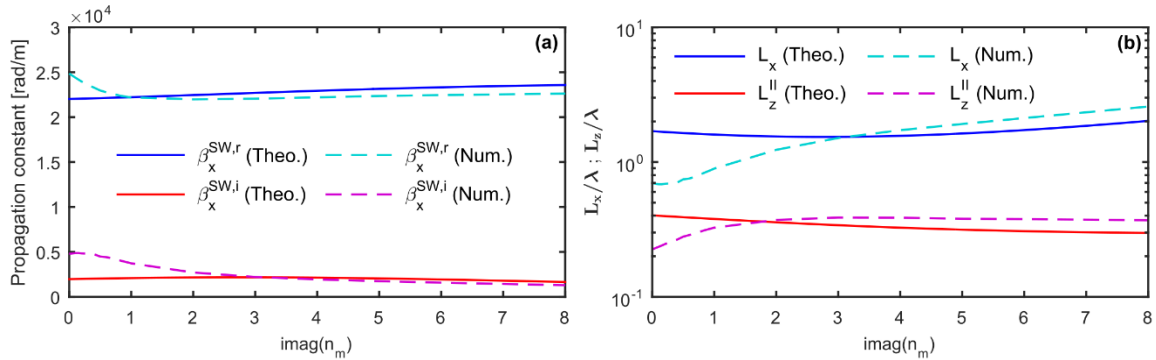


Figure 5.10 Propagation constant of spoof surface wave as a function of the imaginary part of the refractive index of the high permittivity material at 1 THz operation frequency. (a) Real and imaginary parts of the fundamental Spoof surface wave propagation constant. (b) Propagation distance L_x and penetration depth into air L_z^{II} in units of λ . Results are found by solving Equations 5.2 and 5.3 using Newton-Raphson iteration method (solid curves) are compared to those found by COMSOL for a structure without IBC (dashed curves). Here, $d = 50 \mu\text{m}$, $a = 35 \mu\text{m}$, $h = 25 \mu\text{m}$, $\epsilon_0 = 1$ and $\text{real}(n_m) = 10$.

Here, we see that as predicted by the results from Figure 5.9, deviations between the analytic formulation and the numerical results are important for low-loss material as the coupling field

though the notch is strong, resulting in a surface mode propagating at subwavelength distance. However, with high losses, resulting in significant absorption of the field in the notches, the numerical results confirm the analytic one as the IBC approximation becomes valid. In this particular case, both results become similar when the imaginary part of the refractive index is higher than 3, corresponding in a 75% absorption of the field over the distance of a notch $d - a$. Thus, the semi-analytical formulation is valid for subwavelength structure as long as the structure is either made of lossy material or has large notches with non-lossless material. In both cases, one must ensure that the subwavelength condition is respected in order to avoid the effect of diffraction. The limit of this condition can be retrieved by comparing the analytic dispersion relation to numerical results for structures with increasing period d . In Figure 5.11, the propagation constant in function of the period for various operational frequencies is presented. For small period, deviations between the analytic derivation and the numerical results got for a model without IBC are present due to the invalidity of the IBC approximation as previously shown. Both results are then similar for larger periods until the limit $d = 0.4\lambda$, where numerical results start to deviate. Past this point, the surface mode is highly affected by the diffraction due to the large period of the structure. From there, one can quantify these modes as evanescent waves as the field distribution around the interface becomes highly delocalized.

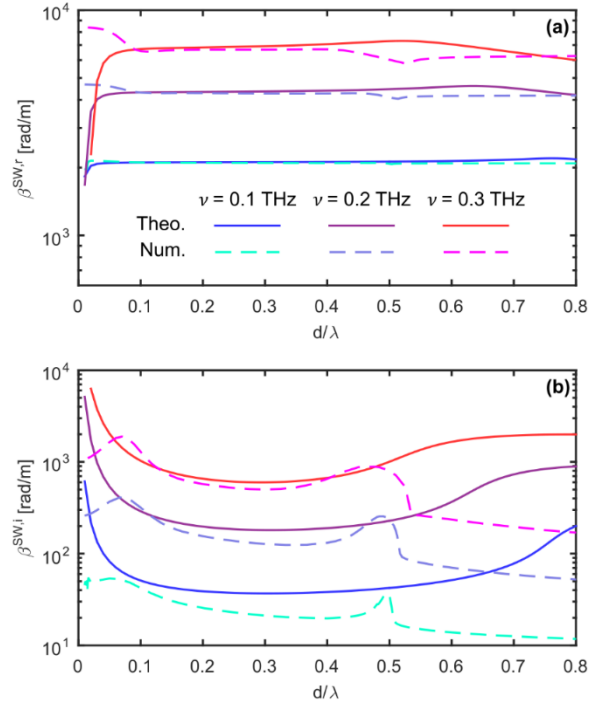


Figure 5.11 Propagation constant of spoof surface wave as a function of the period d in unit of λ at frequencies of 0.1 THz, 0.2 THz, and 0.3 THz. (a) Real and (b) imaginary parts of the fundamental Spoof surface wave propagation constant. Results are found by solving Equations 5.2 and 5.3 using Newton-Raphson iteration method (solid curves) are compared to those found by COMSOL for a structure without IBC (dashed curves). Here, $a = d/2$, $h = 100 \mu\text{m}$, $\varepsilon_0 = 1$, and $n_m = 10 + 5i$.

5.8 Excitation of the spoof surface wave

Earlier in the paper we studied dispersion relation and existence criteria for the novel type of surface waves propagating along all-dielectric corrugated interfaces. In this section we present several strategies for the excitation and experimental observation of such waves. To efficiently excite a spoof surface wave along the corrugated interface one must ensure that the external light source has a component of the electric field perpendicular to the interface, that the fields of an external source overlap strongly with the fields of a surface wave, and, lastly, one has to ensure that the propagation constant of a surface wave is matched with the wavevector component along the interface of the source waves. Note that effective refractive indices of the spoof surface waves described in this work are often somewhat smaller than the refractive index of the filler dielectric

(top cladding). In this case, phase matching between an external light source and a surface wave can be achieved by simply launching a source wave (such as a transverse magnetic gaussian beam) directly from the top cladding onto the corrugated interface at a certain grazing angle θ_0 with respect to the interface:

$$k_0 \cos(\theta_0) = \beta_x^{SW} \quad (5.29)$$

In this case, however, it is difficult to distinguish between the surface wave and reflected source wave due to their virtually collinear propagation. One, therefore, needs to spatially separate the excitation wave from the surface wave. To this end, many simple but inefficient methods can be used to achieve such excitation. Particularly, by using a spatially structured source wave that contains a continuum of wave vectors along the interface (ex. Gaussian beam passed through a small aperture) one can guarantee that the phase matching condition (Equation 5.29) is respected by a small portion of the excitation light, while the rest of it is scattered away from the surface. The main drawback of this type of excitation arrangement is its low efficiency. Examples of such an experimental scheme for the excitation of spoof surface plasmon polaritons [120, 122] include sending the parallel beam along the corrugated interface through a subwavelength aperture. The coupling can be further improved by correcting the momentum mismatch between the excitation waves and the surface wave by using gradient dielectric metastructure [150, 151]. Other waveguide-based couplers can also be exploited to correct the mismatch while localizing the energy near the interface, such as a tapered parallel plate waveguide patterned with a gradient corrugated structure [152]. In Figure 5.12, two of the abovementioned coupling methods are modeled using the COMSOL software, which are respectively the subwavelength aperture (see Figure 5.12 (a)) and the tapered parallel plate waveguide (see Figure 5.12 (b)). In both cases, the excitation source is a transverse magnetic gaussian beam at frequency of 0.24 THz, while the corrugated structure has a period $d = 300 \mu\text{m}$, groove width $a = 50 \mu\text{m}$, groove height $h = 150 \mu\text{m}$, and permittivity constants of $\epsilon_0 = 1$ and $\epsilon_m = 100$. In the first case (see Figure 5.12 (a)), an aperture diffracts and reflects most of the incident wave, while a small fraction of the incident power is coupled into a spoof surface wave. Similarly, in the second case (see Figure 5.12 (b)) spoof surface wave is seen exiting the parallel plate waveguide. By comparing these field distributions to those of the eigen modes of an identical infinitely periodic structure using a full structure simulation shown in insert of Figure 5.12, we confirm that, indeed, a spoof surface wave with the predominant electric field concentration in the gaps is excited by these two methods.

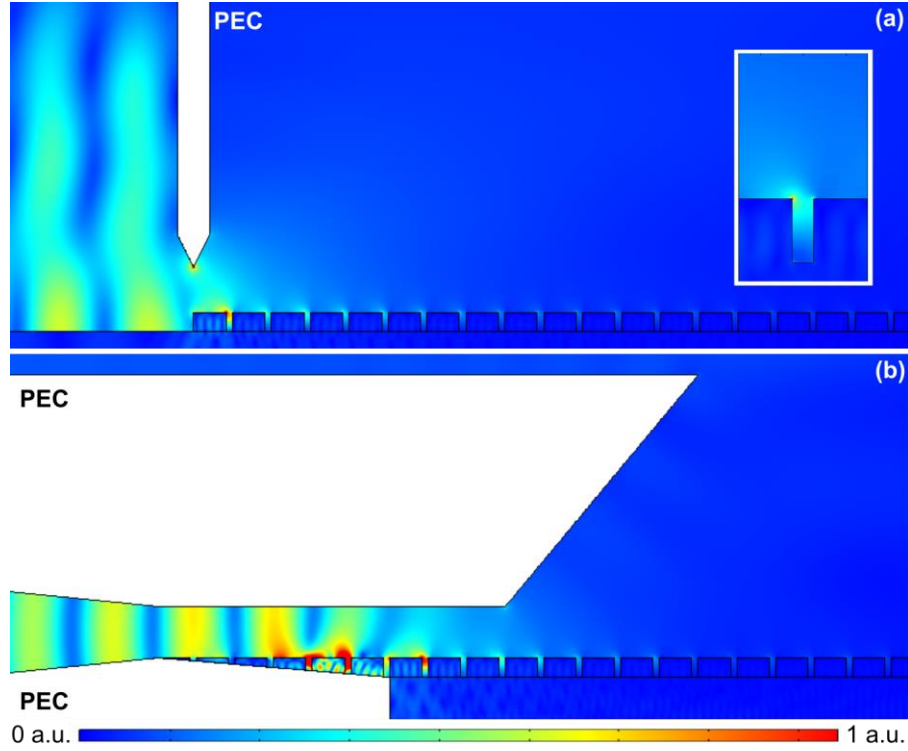


Figure 5.12 Excitation of a spoof surface wave on non-conductive interfaces. (a) Electric field norm distribution when exciting a spoof surface wave using a TM incident gaussian beam incident onto a subwavelength aperture. (b) Electric field norm distribution when exciting a spoof surface wave using a tapered parallel plate waveguide patterned with a corrugated structure. (insert) Distribution of the expected electric field norm in one cell of the periodic structure found with COMSOL for a complete structure without IBC. Operation frequency is 0.24 THz, and the structural parameters are $d = 300 \mu\text{m}$, $a = 50 \mu\text{m}$, $h = 150 \mu\text{m}$, $\epsilon_0 = 1$, and $\epsilon_m = 100$. Both the aperture walls and the walls of a parallel plate waveguide are modeled as a Perfect Electric Conductor.

Finally, for excitation of the spoof surface waves one can use a prism-assisted coupling method, which is widely used for excitation of the surface plasmon polaritons [81, 82, 153]. Within this method, the excitation field, such as a transverse magnetic THz beam, is incident at a certain angle onto one side of a triangular prism with refractive index n_p . The excitation beam is then refracted in the prism, which leads to the beam being incident onto the second facet of the prism at an angle θ_p (with respect to the facet normal). One then places the corrugated structure that supports a surface wave with effective refractive index n_{eff}^{SW} parallel to the second facet of the prism. Finally,

phase matching between the excitation beam and a surface wave at the prism surface can be achieved by the proper choice of an incidence angle such that:

$$n_p \sin(\theta_p) = n_{eff}^{SW} \quad (5.30)$$

As an example, the prism coupling method is demonstrated numerically for the corrugated structure with period $d = 300 \text{ } \mu\text{m}$, groove width $a = 175 \text{ } \mu\text{m}$, groove height $h = 150 \text{ } \mu\text{m}$, and permittivity constants of $\epsilon_0 = 1$ and $\epsilon_m = 100$ operating at 0.18 THz (see Figure 5.13). In this simulation, the incident angle of the source is chosen to respect the phase matching condition (Equation 5.30), where effective refractive index of a surface wave $n_{eff}^{SW} = 1.013$ is found by solving the full structure under COMSOL. The semi-analytical formulation can also be used to retrieve an approximation of the expected effective refractive index $n_{eff}^{SW} = 1.036$. For this choice of the operational parameters, results of a semi-analytical approximation match well the effective refractive index as predicted by the full structure simulation using COMSOL for an infinitely periodic system. This is due to suppression of the electric field in the notches due to geometric anti-resonance in the corrugated structure, a situation when IBC approximation is valid. In Figure 5.13 (a) we, thus, observe resonant excitation of a spoof surface wave. The electric field norm distribution in thus excited spoof surface wave (see Figure 5.13 (b)) matches well the electric field norm distribution as calculated for an infinitely periodic structure (see insert in Figure 5.13 (a)).

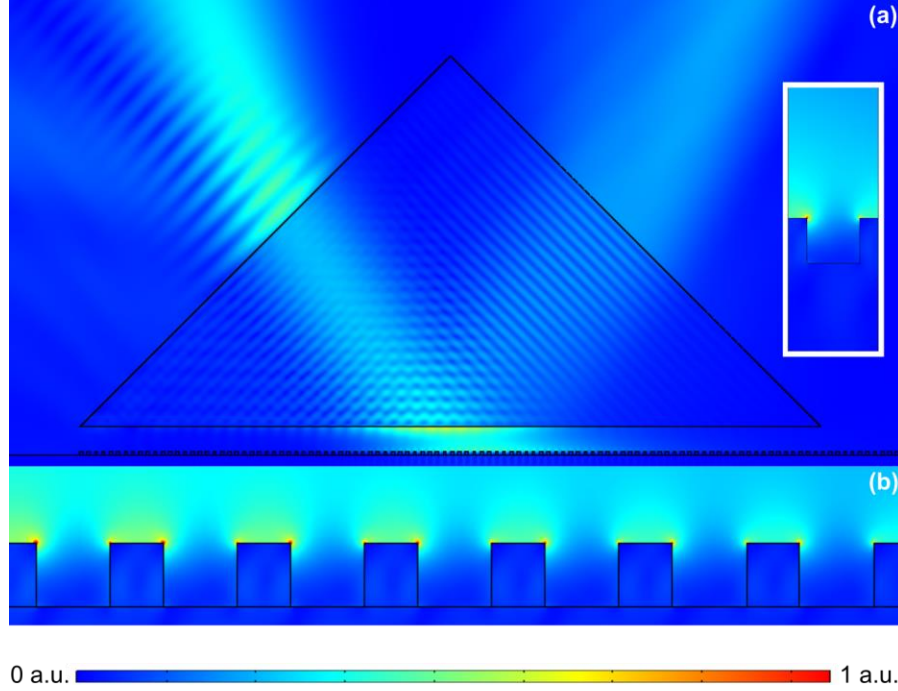


Figure 5.13 Prism-assisted excitation of a spoof surface wave. (a) Electric field norm distribution in the prism-coupled system. (b) Close up: electric field norm distribution in a spoof surface wave excited under the prism. (insert) Distribution of the expected electric field norm in one cell of the periodic structure found with COMSOL for a complete structure without IBC. Simulations are performed at a frequency of 0.18 THz, and the structure parameters $d = 300 \mu\text{m}$, $a = 175 \mu\text{m}$, $h = 150 \mu\text{m}$, $\epsilon_0 = 1$, and $\epsilon_m = 100$, refractive index of the prism is $n_p = 2$.

5.9 Conclusion

In this paper we demonstrate a new type of spoof surface waves that propagate along periodic corrugated surfaces made of non-conducting materials featuring high positive permittivity. Existence of such waves is due to possibility of the electromagnetic energy confinement in the planar groove waveguides limited by the high dielectric permittivity walls. Unlike the case of spoof surface waves on structured metallic surfaces where electromagnetic energy is exponentially fast decreasing into metal, in our case, significant radiation presence is possible in the high dielectric permittivity material. Thus, a careful consideration of radiative effects is important for the proper design of spoof surface waves on the non-conducting surfaces. An analytic derivation of the spoof surface wave dispersion relation is presented in the case of deeply subwavelength period of a

corrugated structure using impedance boundary conditions at the interfaces. Thus, obtained dispersion relation is then verified numerically using COMSOL Multiphysics software on a full system comprising a filler dielectric, a structured high permittivity dielectric, as well as radiation absorbing boundary conditions, and an overall good agreement between semi-analytical theory and numerical simulations is obtained. Finally, we confirmed that there exists a region of design space where spoof surface wave on a non-conducting interface can be tightly confined at such an interface with its transverse size comparable or even smaller than the wavelength of light in the filler dielectric. Additionally, such surface waves can feature propagation distances much longer than their transverse size, thus making such surface waves like the regular guided modes for practical purposes. As spoof surface waves require high dielectric permittivity materials for their experimental realisation, we believe that longer wavelengths spectral ranges (THz, microwave, etc.) are the most suitable for the demonstration of such waves due to abundance of dielectrics with relative permittivity higher than 100.

5.10 Supplemental material

5.10.1 Spatial localization and propagation distance of spoof surface waves

In the grooves (zone I, in Figure 5.1), we have two waves propagating along the z-direction with propagation constant denoted as β_z^I and $-\beta_z^I$. The wave propagating toward the positive z-direction come from the reflection at the bottom of the groove at $z = -h$. Also, the structure in zone I is similar to a waveguide made of two parallel planar materials of permittivity ε_m separated by a dielectric of permittivity ε_0 . Thus, for a TM mode inside the groove waveguide, one can easily solve the Maxwell equations and find the following magnetic and electric components [148]:

$$H_y^{I+} = A^+ \cos(k_x^I x) e^{i\beta_z^I z} \quad (5.31)$$

$$E_z^{I+} = -iA^+ \frac{k_x^I}{\varepsilon_0 k_0} \sin(k_x^I x) e^{i\beta_z^I z} \quad (5.32)$$

$$E_x^{I+} = A^+ \frac{\beta_z^I}{\varepsilon_0 k_0} \cos(k_x^I x) e^{i\beta_z^I z} \quad (5.33)$$

where A^+ is a constant and where the relation between k_x^I and β_z^I is given by:

$$k_x^I = \sqrt{\varepsilon_0 k_0^2 - (\beta_z^I)^2} \quad (5.34)$$

Here for simplicity, we only consider even modes of a groove waveguide as described by Equations 5.31-5.33, that also comprise the fundamental mode. While the formulation for the odd modes ($H_y^{I+} \sim \sin(k_x^I x)$) can be easily derived, in this work we do not present it for the sake of brevity. Moreover, in practical applications, one would most probably favor the fundamental even mode, as it is the easiest to be realised experimentally.

We also have three impedance boundary conditions in the groove to respect at the interfaces $x = a/2$, $x = -a/2$ and $z = -h$:

$$H_y^{I+}|_{x=a/2} = -\sqrt{\varepsilon_m} E_z^{I+}|_{x=a/2} \quad (5.35)$$

$$H_y^{I+}|_{x=-a/2} = \sqrt{\varepsilon_m} E_z^{I+}|_{x=-a/2} \quad (5.36)$$

$$H_y^{I+}|_{z=-h} = -\sqrt{\varepsilon_m} E_x^{I+}|_{z=-h} \quad (5.37)$$

Using the impedance boundary conditions 5.35 with the expressions 5.31 and 5.32, we get:

$$\cos\left(k_x^I \frac{a}{2}\right) = i\sqrt{\varepsilon_m} \frac{k_x^I}{\varepsilon_0 k_0} \sin\left(k_x^I \frac{a}{2}\right) \quad (5.38)$$

$$\Rightarrow k_x^I \tan(k_x^I a/2) = -i \frac{k_0 \varepsilon_0}{\sqrt{\varepsilon_m}} \quad (5.39)$$

where Equation 5.39 with the relation 5.34 can be simplified as follows when the argument $k_x^I a/2$ is small:

$$(k_x^I)^2 \simeq -i \frac{2 \varepsilon_0 k_0}{a \sqrt{\varepsilon_m}} \quad (5.40)$$

$$\Rightarrow \beta_z^I = \sqrt{\varepsilon_0 k_0^2 - (k_x^I)^2} \simeq \sqrt{\varepsilon_0} k_0 + i \frac{\sqrt{\varepsilon_0}}{a \sqrt{\varepsilon_m}} \quad (5.41)$$

A numerical method such as the Newton-Raphson iteration method can also be used to find the expression of β_z^I from Equation 5.34 and 5.39. Moreover, the other wave propagating toward the negative z direction has a propagation constant that corresponds to $-\beta_z^I$. The magnetic and electric components are then given by:

$$H_y^{I-} = A^- \cos(k_x^I x) e^{-i\beta_z^I z} \quad (5.42)$$

$$E_z^{I-} = -iA^- \frac{k_x^I}{\varepsilon_0 k_0} \sin(k_x^I x) e^{-i\beta_z^I z} \quad (5.43)$$

$$E_x^{I-} = -A^- \frac{\beta_z^I}{\varepsilon_0 k_0} \cos(k_x^I x) e^{-i\beta_z^I z} \quad (5.44)$$

where A^- is a constant. The total electric and magnetic components in the first zone can be written as the combination of the two waves propagating along the z -direction:

$$H_y^I = \cos(k_x^I x) [A^+ e^{i\beta_z^I z} + A^- e^{-i\beta_z^I z}] \quad (5.45)$$

$$E_z^I = -i \frac{k_x^I}{\varepsilon_0 k_0} \sin(k_x^I x) [A^+ e^{i\beta_z^I z} + A^- e^{-i\beta_z^I z}] \quad (5.46)$$

$$E_x^I = \frac{\beta_z^I}{\varepsilon_0 k_0} \cos(k_x^I x) [A^+ e^{i\beta_z^I z} - A^- e^{-i\beta_z^I z}] \quad (5.47)$$

In addition, the relation between the coefficients A^+ and A^- can be found with the impedance boundary condition at $z = -h$ and Equations 5.45 and 5.47:

$$A^+ e^{-i\beta_z^I h} \left(\frac{\beta_z^I}{\varepsilon_0 k_0} + \frac{1}{\sqrt{\varepsilon_m}} \right) = A^- e^{i\beta_z^I h} \left(\frac{\beta_z^I}{\varepsilon_0 k_0} - \frac{1}{\sqrt{\varepsilon_m}} \right) \quad (5.48)$$

$$\Rightarrow A^+ = A^- e^{2i\beta_z^I h} \left(\frac{\sqrt{\varepsilon_m} \beta_z^I - \varepsilon_0 k_0}{\sqrt{\varepsilon_m} \beta_z^I + \varepsilon_0 k_0} \right) \quad (5.49)$$

Because of the impedance boundary condition and radiative loss at the waveguide boundaries, the amplitude of the wave propagating toward the positive z direction is smaller than the wave propagating toward the bottom of the cavity. Also, the groove depth h controls the phase difference between these two waves. These observations suggest that the groove depth will have a significant impact on the complex dispersion relation of the spoof surface wave supported by the corrugated surface.

Next, the magnetic and electric components of the wave propagating along the x axis in the region above the surface ($z > 0$) are given by:

$$H_y^{II} = \sum_n B_n e^{i\beta_x^{II,n} x} e^{ik_z^{II,n} z} \quad (5.50)$$

$$E_x^{II} = \sum_n B_n \frac{k_z^{II,n}}{\varepsilon_0 k_0} e^{i\beta_x^{II,n} x} e^{ik_z^{II,n} z} \quad (5.51)$$

$$E_z^{II} = -\sum_n B_n \frac{\beta_x^{II,n}}{\varepsilon_0 k_0} e^{i\beta_x^{II,n} x} e^{ik_z^{II,n} z} \quad (5.52)$$

$$(k_z^{II,n})^2 = \varepsilon_0 k_0^2 - (\beta_x^{II,n})^2; \quad \beta_x^{II,n} = \beta_x^{SW} + G_n \quad (5.53)$$

where $G_n = 2\pi n/d$ comes from the Bloch periodicity. At $z = 0$, we must match the components from zone I and II above the grooves $x \in (-a/2, a/2)$ and respect the impedance boundary condition otherwise for $x \in (-d/2, -a/2) \cup (a/2, d/2)$. For the first case above the grooves, we have:

$$H_y^{II}|_{z=0} = H_y^I|_{z=0} \quad (5.54)$$

$$E_x^{II}|_{z=0} = E_x^I|_{z=0} \quad (5.55)$$

Then, we have for the impedance boundary condition at the interface at $x \in (-d/2, -a/2) \cup (a/2, d/2)$:

$$H_y^{II}|_{z=0} = -\sqrt{\varepsilon_m} E_x^{II}|_{z=0} \quad (5.56)$$

Here, to find the expression of the effective refractive index of the spoof surface waves, one must solve the previous equations and conditions. To begin, a first relation between the coefficients B_n , A^+ and A^- can be found from relations 5.55 and 5.56:

$$E_x^{II}|_{z=0} = \sum_n B_n \frac{k_z^{II,n}}{\varepsilon_0 k_0} e^{i\beta_x^{II,n} x} = \begin{cases} A \frac{\beta_z^I}{\varepsilon_0 k_0} \cos(k_x^I x), & x \in \left(-\frac{a}{2}, \frac{a}{2}\right) \\ -\frac{1}{\sqrt{\varepsilon_m}} \sum_n B_n e^{i\beta_x^{II,n} x}, & x \in \left(-\frac{d}{2}, -\frac{a}{2}\right) \cup \left(\frac{a}{2}, \frac{d}{2}\right) \end{cases} \quad (5.57)$$

where $A = A^+ - A^-$. In the limit of $d \ll \lambda$, only $n = 0$ is of importance. Thus, we get:

$$E_x^{II}|_{z=0} = B_0 k_z^{SW,II} e^{i\beta_x^{SW} x} = \begin{cases} A \beta_z^I \cos(k_x^I x), & x \in \left(-\frac{a}{2}, \frac{a}{2}\right) \\ -\frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} B_0 e^{i\beta_x^{SW} x}, & x \in \left(-\frac{d}{2}, -\frac{a}{2}\right) \cup \left(\frac{a}{2}, \frac{d}{2}\right) \end{cases} \quad (5.58)$$

$$\Rightarrow k_z^{SW,II} \int_{-d/2}^{d/2} e^{i\beta_x^{SW} x} dx = \beta_z^I \frac{A}{B_0} \int_{-a/2}^{a/2} \cos(k_x^I x) dx - \frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} \left[\int_{-\frac{a}{2}}^{-\frac{d}{2}} e^{i\beta_x^{SW} x} dx + \int_{\frac{a}{2}}^{\frac{d}{2}} e^{i\beta_x^{SW} x} dx \right] \quad (5.59)$$

$$\Rightarrow k_z^{SW,II} \sin\left(\beta_x^{SW} \frac{d}{2}\right) = \frac{A}{B_0} \frac{\beta_z^I \beta_x^{SW}}{k_x^I} \sin\left(k_x^I \frac{a}{2}\right) - \frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} \left[\sin\left(\beta_x^{SW} \frac{d}{2}\right) - \sin\left(\beta_x^{SW} \frac{a}{2}\right) \right] \quad (5.60)$$

$$\Rightarrow B_0 = A \frac{\beta_z^I \beta_x^{SW}}{k_x^I} \frac{\sin\left(k_x^I \frac{a}{2}\right)}{\left(\frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} + k_z^{SW,II}\right) \sin\left(\beta_x^{SW,II} \frac{d}{2}\right) - \frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} \sin\left(\beta_x^{SW} \frac{a}{2}\right)} \quad (5.61)$$

A third relation between A^+ , A^- and B_0 can be found with the continuity condition of the magnetic component at $z = 0$ represented by Equation 5.54:

$$\sum_n B_n e^{i\beta_x^{II,n}x} = (A^+ + A^-) \cos(k_x^I x) \quad (5.62)$$

In the limit of $d \ll \lambda$, only $n = 0$ is of importance. So, we get:

$$B_0 e^{i\beta_x^{SW}x} = (A^+ + A^-) \cos(k_x^I x) \quad (5.63)$$

$$\Rightarrow B_0 \int_{-a/2}^{a/2} e^{i\beta_x^{SW}x} dx = (A^+ + A^-) \int_{-a/2}^{a/2} \cos(k_x^I x) dx \quad (5.64)$$

$$\Rightarrow B_0 \frac{1}{\beta_x^{SW}} \sin\left(\beta_x^{SW} \frac{a}{2}\right) = (A^+ + A^-) \frac{1}{k_x^I} \sin\left(k_x^I \frac{a}{2}\right) \quad (5.65)$$

$$\Rightarrow B_0 = (A^+ + A^-) \frac{\beta_x^{SW}}{k_x^I} \frac{\sin\left(k_x^I \frac{a}{2}\right)}{\sin\left(\beta_x^{SW} \frac{a}{2}\right)} \quad (5.66)$$

At this point we have three unknown constants A^+ , A^- and B_0 with three equations 5.49, 5.61, and 5.66. Thus, β_x^{SW} can now be solved:

$$(A^+ + A^-) \frac{\beta_x^{SW}}{k_x^I} \frac{\sin\left(k_x^I \frac{a}{2}\right)}{\sin\left(\beta_x^{SW} \frac{a}{2}\right)} = (A^+ - A^-) \frac{\beta_z^I \beta_x^{SW}}{k_x^I} \frac{\sin\left(k_x^I \frac{a}{2}\right)}{\left(\frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} + k_z^{SW,II}\right) \sin\left(\beta_x^{SW} \frac{d}{2}\right) - \frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} \sin\left(\beta_x^{SW} \frac{a}{2}\right)} \quad (5.67)$$

$$\Rightarrow \left(\frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} + k_z^{SW,II}\right) \frac{\sin\left(\beta_x^{SW} \frac{d}{2}\right)}{\sin\left(\beta_x^{SW} \frac{a}{2}\right)} = \beta_z^I \frac{i\sqrt{\varepsilon_m} \beta_z^I \tan(\beta_z^I h) - \varepsilon_0 k_0}{\sqrt{\varepsilon_m} \beta_z^I - i\varepsilon_0 k_0 \tan(\beta_z^I h)} + \frac{\varepsilon_0 k_0}{\sqrt{\varepsilon_m}} \quad (5.68)$$

where $k_z^{SW,II} = \sqrt{\varepsilon_0 k_0^2 - (\beta_x^{SW})^2}$ and $\beta_x^{SW} = k_0 n_{eff}^{SW}$. Up to now, we found analytic expressions of the dispersion relations of the wave propagating in the grooves (Equation 5.39) and the spoof surface waves propagating along the interface (Equation 5.68). One can then use numerical method such as the Newton-Raphson iteration method to solve for β_z^I and β_x^{SW} . However, further simplifications can be applied under specific conditions. To begin with, the dispersion relation can be greatly simplified while considering an ideal case where the corrugated structure is made of material with very high positive permittivity $\varepsilon_m \rightarrow +\infty$:

$$\beta_x^{SW} = \sqrt{\varepsilon_0 k_0^2 + \left(\beta_z^I \tan(\beta_z^I h) \frac{\sin\left(\beta_x^{SW} \frac{a}{2}\right)}{\sin\left(\beta_x^{SW} \frac{d}{2}\right)}\right)^2} \quad (5.69)$$

Additionally, further simplifications can be done for a subwavelength corrugation $\beta_x^{SW} d \ll 1$:

$$\beta_x^{SW} = \sqrt{\varepsilon_0 k_0^2 + \left(\beta_z^I \tan(\beta_z^I h) \left(\frac{a}{d}\right)\right)^2} \quad (5.70)$$

Both equations can be represented as universal functions of several non-dimensional variables, which will help to identify the relation of each parameter of the structured material d , a , h , $\sqrt{\varepsilon_0}$, and $\sqrt{\varepsilon_m}$ on the dispersion relations. In fact, we can show that we can represent the effective refractive index of the waves n_{eff}^I and n_{eff}^{SW} as a function of these following non-dimensional variables $hk_0\sqrt{\varepsilon_0}$, $ak_0\sqrt{\varepsilon_0}$, $dk_0\sqrt{\varepsilon_0}$, and $\sqrt{\varepsilon_0}/\sqrt{\varepsilon_m}$:

$$\frac{k_x^I}{\sqrt{\varepsilon_0}k_0} \tan\left(\frac{k_x^I}{\sqrt{\varepsilon_0}k_0} \frac{ak_0\sqrt{\varepsilon_0}}{2}\right) = -i \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} \quad (5.71)$$

$$\Rightarrow \frac{n_{eff}^I}{\sqrt{\varepsilon_0}} = \pm \sqrt{1 - \left(\frac{k_x^I}{\sqrt{\varepsilon_0}k_0}\right)^2} \quad (5.72)$$

$$\left(\frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} + \frac{k_z^{SW,II}}{\sqrt{\varepsilon_0}k_0}\right) \frac{\sin\left(\frac{n_{eff}^{SW}}{\sqrt{\varepsilon_0}} \frac{dk_0\sqrt{\varepsilon_0}}{2}\right)}{\sin\left(\frac{n_{eff}^{SW}}{\sqrt{\varepsilon_0}} \frac{ak_0\sqrt{\varepsilon_0}}{2}\right)} = i \frac{\beta_z^I}{\sqrt{\varepsilon_0}k_0} \frac{\tan\left(\frac{n_{eff}^I}{\sqrt{\varepsilon_0}} hk_0\sqrt{\varepsilon_0}\right) + i \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} \frac{n_{eff}^I}{n_{eff}^I}}{1 - i \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} \frac{n_{eff}^I}{n_{eff}^I} \tan\left(\frac{n_{eff}^I}{\sqrt{\varepsilon_0}} hk_0\sqrt{\varepsilon_0}\right)} + \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_m}} \quad (5.73)$$

$$\Rightarrow \frac{k_z^{SW,II}}{\sqrt{\varepsilon_0}k_0} = \pm \sqrt{1 - \left(\frac{n_{eff}^{SW}}{\sqrt{\varepsilon_0}}\right)^2} \quad (5.74)$$

5.10.2 Wave propagating in corrugated coating

Here we derive dispersion relation of leaky waves propagating along the layer interfaces in a three-layer system. The individual layers are characterised by permittivity constants ε_0 , ε_c , and ε_m , where the middle layer is anisotropic and described by a diagonal permittivity tensor $\varepsilon_c = (\varepsilon_c^x, \varepsilon_c^y, \varepsilon_c^z)$. In our derivations we use a standard transfer matrix theory for TM polarized waves adapted to treat anisotropic materials having two of its symmetry axis aligned with the planar interfaces. Assuming only outgoing planewaves $B \cdot \exp(i\beta x - ik_0^z z)$ in the top cladding, and $A \cdot \exp(i\beta x + ik_m^z z)$ in the bottom claddings, then the amplitudes of the two outgoing waves are related by a 2x2 transfer matrix T :

$$\begin{bmatrix} A \\ 0 \end{bmatrix} = T \begin{bmatrix} 0 \\ B \end{bmatrix}; \quad T = M_{c,m} M_{0,c} \quad (5.75)$$

$$M_{c,m} = \frac{1}{2} \begin{bmatrix} (1+q)e^{i\phi} & (1-q)e^{-i\phi} \\ (1-q)e^{i\phi} & (1+q)e^{-i\phi} \end{bmatrix} \quad (5.76)$$

$$M_{0,c} = \frac{1}{2} \begin{bmatrix} 1+p & 1-p \\ 1-p & 1+p \end{bmatrix} \quad (5.77)$$

where

$$p = \frac{\varepsilon_c^x k_a^z}{\varepsilon_0 k_c^z}, \quad q = \frac{\varepsilon_m k_c^z}{\varepsilon_c^x k_m^z}, \quad \phi = k_c^z h \quad (5.78)$$

And the transverse wave vector in the isotropic and anisotropic layers are given by:

$$k_{0,m}^z = \sqrt{\varepsilon_{0,m} k_0^2 - \beta^2} \quad (5.79)$$

$$k_c^z = \sqrt{\varepsilon_c^x k_0^2 - (\varepsilon_c^x / \varepsilon_c^z) \beta^2} \quad (5.80)$$

One can then readily solve the matrix Equation 5.75 to find the equation for the leaky mode dispersion relation:

$$\frac{1+pq}{p+q} = i \tan \phi \quad (5.81)$$

In the case where $|\varepsilon_m| \rightarrow \infty$, Equation 5.81 can be solved analytically to give:

$$\varepsilon_{eff} \simeq \varepsilon_0 \left(1 + \frac{a}{d} \tan^2 \left(k_0 \sqrt{\frac{d}{a}} \varepsilon_0 h \right) \right) \quad (5.82)$$

5.10.3 Details of COMSOL simulations

To validate the analytic dispersion relation given by Equations 5.2 and 5.3 along with the study of the validity of the IBC, the finite element software COMSOL Multiphysics 5.5 has been used to numerically solve the electromagnetic surface waves supported by the corrugated structure. All the simulations were performed in the frequency domain, where one period of the structure is modeled together with the Floquet periodic conditions at $x = \pm d/2$. This condition along with the COMSOL's eigenfrequency study step allows us to find the complex eigen frequency $\nu_{num}(\beta_x)$ that corresponds to a given real propagation constant β_x . For the structure using IBC, a simple domain made of the filler dielectric of dielectric permittivity ε_0 representing the combination of region I and II is delimited by the periodic conditions (region I) and IBC inside the groove (region II). The region above $z = 0$, which extends up to multiple times the operational wavelengths, is terminated with a PML (perfect matched layers) domain and scattering boundary condition at the outer boundary. For the full structure (without IBC), all the three zones illustrated in Figure 5.1

along with the high dielectric permittivity material ε_m in zone III and below $z = -h$ is included into simulation cell. In this case, the computational cell is terminated both from the top and bottom with the PML domains and scattering boundary conditions.

As mentioned earlier, the eigenfrequency search method was used to numerically find the complex dispersion relation $\nu_{num}(\beta_x) = \nu_{num}^r(\beta_x) + i\nu_{num}^i(\beta_x)$ of the supported surface waves, where β_x is real and specified in the Floquet boundary conditions. In practical applications, however, one is rather interested in the complex propagation constant of the mode $\beta_x^{SW}(\nu) = \beta_x^{SW,r}(\nu) + i\beta_x^{SW,i}(\nu)$ for the pure real frequencies ν . Thus, for practical applications, and in order to compare semi-analytic dispersion relation given by Equations 5.2 and 5.3 along with the numerical ones, one has to know how to transform dispersion relation in terms of a complex frequency $\nu_{num}(\beta_x)$ given by COMSOL into dispersion relations in terms of a complex propagation constant $\beta_x^{SW}(\nu)$. Particularly, assuming that eigen frequency $\nu_{num}(\beta_x)$ (as computed by COMSOL) can be computed for any propagation constant β_x , we then look for the complex propagation constants β_x that result in the purely real eigenfrequencies:

$$\nu_{num}^i(\beta_x^r, \beta_x^i) = 0 \quad (5.83)$$

Multiple methods can be used to solve Equation 5.83. As example, one could start with a purely real propagation constant $\beta_{x,0} = (\beta_x^r, 0)$ that would result in the complex eigenfrequency $\nu_{num}(\beta_{x,0})$, and then use an iterative method (like the method of secants used in our work) to find the corresponding imaginary part of the propagation constant β_x^i so that the complex $\beta_x = (\beta_x^r, \beta_x^i)$ would result in the purely real eigen frequency (Equation 5.83). Particularly, for the n^{th} iteration one can use:

$$\beta_{x,n+1}^i = \beta_{x,n}^i - \nu_{num}^i(\beta_x^r, \beta_{x,n}^i) \frac{\beta_{x,n}^i - \beta_{x,n-1}^i}{\nu_{num}^i(\beta_x^r, \beta_{x,n}^i) - \nu_{num}^i(\beta_x^r, \beta_{x,n-1}^i)} \quad (5.84)$$

Author contributions

Writing, Mathieu Poulin and Maksim Skorobogatiy; Simulations and figures, Mathieu Poulin. All authors read and approved the final manuscript.

CHAPITRE 6 DISCUSSION GÉNÉRALE

La rédaction des deux articles présentés dans les Chapitres 4 et 5 a permis de définir la problématique soulevée dans ce projet de maîtrise concernant le support de modes de surface localisés dans la gamme spectrale des térahertz, de produire une revue critique de la littérature, de trouver une solution innovante basée sur la conception d'un métamatériau non conducteur, d'effectuer une caractérisation rigoureuse de ce dernier ainsi que de proposer des méthodes d'excitation. En revanche, bien que ces démarches théoriques et numériques proposent l'existence d'un nouveau type de modes de surface, leurs implications réelles ainsi que la reproduction expérimentale de ce métamatériau demeurent des questions peu abordées dans les articles précédents. Ainsi, ce chapitre propose du matériel supplémentaire visant à convaincre les lecteurs du potentiel de ces modes de surface dans le développement d'applications œuvrant dans la plage spectrale des térahertz ainsi que de leurs reproductions dans un contexte expérimental. Pour ce faire, la définition d'un détecteur à amplitude, utilisée lors de la revue de la littérature (Chapitre 4), et la théorie des modes de surface sur le métamatériau non conducteur (Chapitre 5) sont combinées pour la proposition d'un capteur théorique simplifié œuvrant dans les térahertz. Ensuite, une méthode de fabrications de ces métamatériaux est proposée. Enfin, une méthodologie expérimentale pour l'excitation des modes de surface discutés est développée.

6.1 Caractérisation théorique des modes de surface pour les applications de détections dans la gamme spectrale des térahertz

On présente dans cette section un exemple théorique d'un détecteur exploitant l'excitation de modes de surface à l'interface entre le métamatériau non conducteur et une substance à analyser. La sensibilité théorique d'un tel capteur capable de détecter la variation de l'indice de réfraction d'intérêt en fonction des pertes par propagation du mode, donnée par l'Équation 4.6 du Chapitre 4, est aussi présentée.

Pour commencer, on considère un métamatériau tel qu'illustré à la Figure 5.1 (a) correspondant à une surface structurée de céramique TiO_2 ($\epsilon_m = 100$), où une substance à phase gazeuse possédant un indice de réfraction $\epsilon_0 = \epsilon_a = 1$ est située à la surface ainsi que dans les rainures. Ici, on suppose que les approximations des conditions d'impédance aux interfaces sont valides. Ainsi, la relation de dispersion analytique (Équations 5.2 and 5.3) peut être utilisée pour évaluer les propriétés des modes de surface théoriques pouvant être supportés à l'interface entre le métamatériau non conducteur et la substance à analyser, telles que la distance de propagation

typique (Équation 5.9) ainsi que la taille modale des modes de surface dans la substance (Équation 5.10). Par la suite, avec l'aide de ces outils, la conception ingénieuse du métamatériau se base sur un système d'optimisation avec contraintes, où l'objectif est de maximiser la sensibilité du détecteur en fonction des paramètres de la structure. Or, puisque ce capteur demande la propagation d'une onde de surface, une contrainte concernant le support de quasi-ondes de surface pouvant se propager est définie comme suit :

$$L_x(\omega) > L_z^1(\omega) \quad (6.1)$$

Afin de répondre à cet objectif, les paramètres suivants sont proposés pour le support de modes de surface pour une plage de fréquences se situant entre 0.1 THz et 1.0 THz : $d = 40 \mu\text{m}$, $a = 20 \mu\text{m}$ et $h = 20 \mu\text{m}$. La Figure 6.1 illustre les propriétés de ces modes de surface ainsi que la sensibilité théorique du capteur en fonction de la fréquence d'opération.

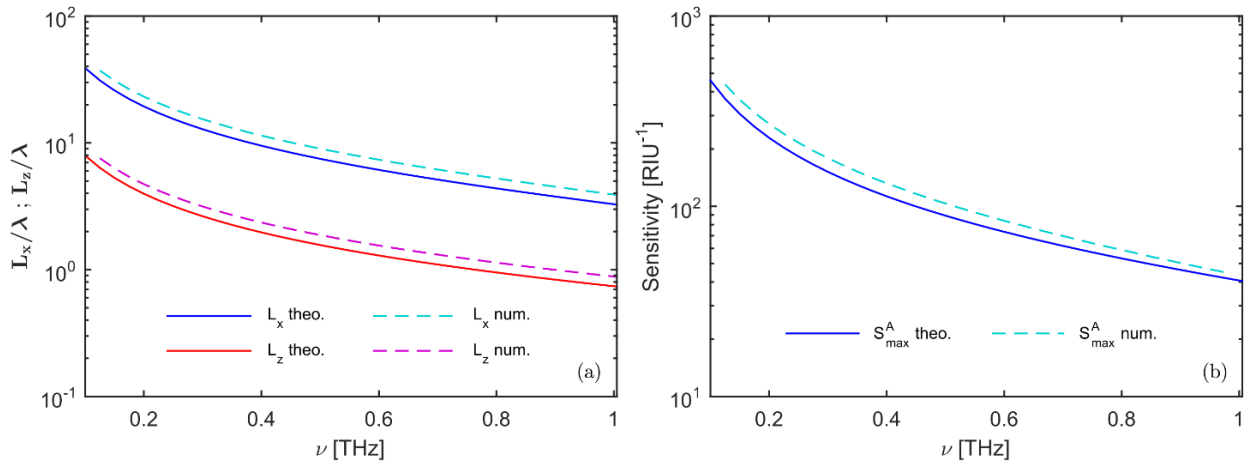


Figure 6.1 (a) Distance de propagation théorique L_x et taille modale L_z des modes de surface en fonction de la fréquence ν . (b) Sensibilité théorique du détecteur en fonction de la fréquence d'opération. Des résultats numériques obtenus à l'aide du logiciel COMSOL accompagnent les valeurs analytiques pour la structure où $d = 40 \mu\text{m}$, $a = 20 \mu\text{m}$, $h = 20 \mu\text{m}$, $\varepsilon_0 = 1$, et $\varepsilon_m = 100$.

La Figure 6.1 (a) illustre les tailles caractéristiques des modes de surface supportés par le métamatériau non conducteur. On observe, dans un premier temps, que ces modes correspondent à des quasi-ondes de surface, où la distance de propagation L_x est 5 fois plus grande que la taille modale dans la substance L_z . Dans un deuxième temps, selon les résultats, la distance de propagation peut atteindre jusqu'à 10 centimètres, permettant de maximiser la sensibilité du capteur telle qu'illustrée dans la Figure 6.1 (b). La taille modale, dans un dernier temps, peut aussi

atteindre des dimensions inférieures à la longueur d'onde d'opération, permettant la conception d'un capteur compact.

Ce type de capteur simplifié correspond à une alternative viable aux détecteurs basés sur la résonance de modes de surface. Ces derniers détectent la variation de l'indice de réfraction d'une substance selon la variation de la fréquence d'excitation d'un mode de résonance, où la sensibilité est définie par la capacité à détecter une variation de l'indice de réfraction (en unité RIU) selon la variation de la fréquence de résonance (en unité fréquentielle). Ainsi, un système de spectroscopie dans le domaine du temps pour le régime spectral des térahertz est nécessaire pour la détection de variations. Dans la littérature, de tels systèmes utilisent généralement des métamatériaux métalliques pour le support des modes de résonances ainsi qu'un prisme de couplage pour l'excitation des quasi-ondes de surface à l'aide d'impulsions incidentes térahertz, permettant d'obtenir des sensibilités de l'ordre de 0.5 THz/RIU [154]. Une sensibilité de 2.27 THz/RIU a aussi été démontrée numériquement par l'excitation de modes supérieurs de surface pour une configuration similaire [83]. Ainsi, le capteur à base de détection d'amplitude proposé dans cette section, pouvant atteindre une sensibilité maximale de 460 RIU⁻¹, correspond à une alternative viable pour sa haute sensibilité maximale à la variation d'indices de réfraction. Il est à noter que la définition de la sensibilité de ce détecteur théorique à amplitude diffère des définitions utilisées pour les systèmes basés sur la résonance des modes de surface, où les unités sont généralement exprimées en THz/RIU ou en θ /RIU, où θ est l'angle d'incidence d'une source d'excitation. Ici, le capteur à amplitude permet de caractériser la variation de la partie imaginaire de l'indice de réfraction effectif du mode $\delta\alpha$ en fonction de la variation de l'indice de réfraction de la substance δn_a . Puisque la sensibilité dépend de la longueur du détecteur, la sensibilité peut être exprimé en RIU/RIU par mètre. Or, puisque la sensibilité maximale de ce type de détecteur est obtenue pour une longueur équivalente à la distance de propagation de l'onde de surface, soit $L_{max} = 1/\alpha$, il est usuel d'exprimer la sensibilité maximale du détecteur à amplitude en RIU⁻¹. Ainsi, il est préférable de comparer cette haute sensibilité obtenue pour ce détecteur à amplitude avec ceux développés dans le Chapitre 4. En effet, à partir des résultats présentés dans les Figures 4.7-4.12, on constate que les détecteurs à amplitude exploitant la propagation d'ondes de surface aux interfaces entre un diélectrique et un matériau fonctionnel (matériau conducteur, matériau polaire, matériau absorbant, graphène et métamatériau métallique) présentent de faibles sensibilités (allant jusqu'à 10 RIU⁻¹). Le métamatériau non conducteur proposé dans ce mémoire est donc un support de modes de surface

flexible, pratique et innovant pour le domaine de la détection œuvrant dans la gamme spectrale des térahertz.

6.2 Technique de fabrication expérimentale de la surface structurée non conductrice

La caractérisation du métamatériau développée dans le Chapitre 5 propose la structuration de surfaces non conductrices pour le support de modes de surface dans la plage fréquentielle des térahertz. La possibilité de remplacer les métaux par des diélectriques, tels que des céramiques, lors de la conception de métamatériaux correspond à une solution intéressante ayant beaucoup de potentiels. Or, pour être viable expérimentalement, il est nécessaire d'identifier des méthodes de fabrications afin de pouvoir produire des rainures précises sur une surface diélectrique. De plus, la caractérisation des limites de la relation de dispersion analytique présentée dans le Chapitre 5.7 demande que la période de la structure soit inférieure à la longueur d'onde d'opération ($d < 0,4\lambda$). Pour une fréquence minimale de 0,1 THz, ce dernier critère demande alors une période maximale de 1200 micromètres. De telles dimensions peuvent aisément être produites avec précision à l'aide de méthodes de microfabrications qui sont généralement utilisées lors de la production de métamatériaux métalliques. Certaines de ces méthodes peuvent aussi être appliquées pour la microfabrication de structures diélectriques. Par exemple, la lithographie, suivie d'un dépôt de céramique par faisceau électronique, puis terminé par une libération chimique permettent la fabrication d'un métamatériau correspondant à une structure périodique de cylindre de TiO_2 [155]. La gravure par ion avec masque peut aussi être exploitée pour obtenir des surfaces structurées en céramique [156]. Finalement, d'autres méthodes alternatives, telles que la compression à chaud de poudres de céramiques et l'usinage mécanique de surfaces solides peuvent aussi être utilisées [157]. Dans ce qui suit, une technique de fabrication basée sur la compression de poudres de céramiques à l'aide de moules obtenus par impression 3D est proposée pour une fabrication simple du métamatériau non conducteur.

L'impression 3D offre la possibilité de concevoir diverses formes à l'aide de filaments plastiques chauffés. La tête d'impression peut se déplacer avec précision dans l'espace afin de produire des couches successives. Les dimensions minimales des filaments déposées peuvent atteindre une épaisseur et une largeur de respectivement 0,1 mm et 0,2 mm. Ces impressions peuvent ainsi servir à produire des moules, dans lesquelles une poudre de céramiques peut être déposée ainsi que

compressée afin d'obtenir un métamatériau non conducteur. Dans l'optique de fabriquer une surface structurée en céramique telle que présentée dans le Chapitre 5, deux moules ont été conçus, puis fabriqués à l'aide d'une imprimante 3D. La Figure 6.2 illustre les deux moules nécessaires pour la compression du métamatériau non conducteur ainsi que leurs dimensions.

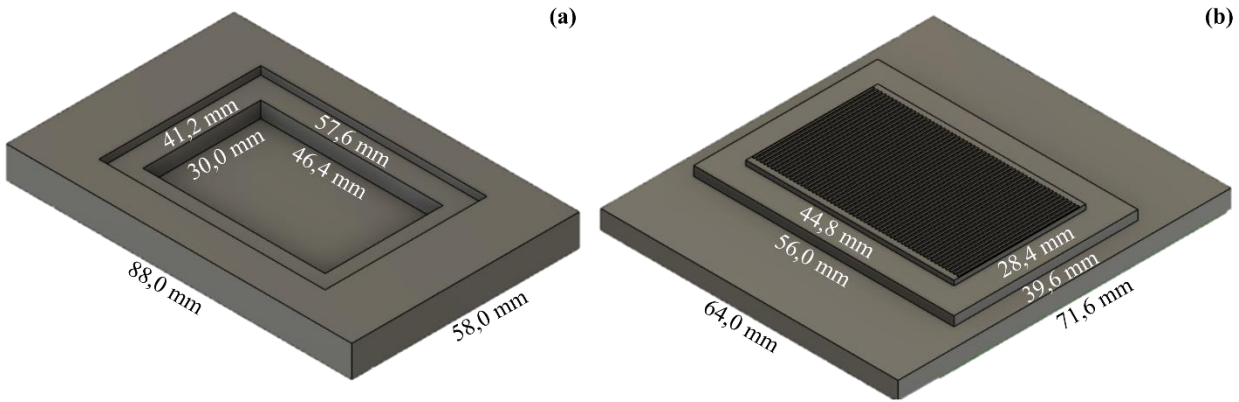


Figure 6.2 Modèles et dimensions des deux moules pour la compression de la poudre de céramiques en une surface structurée de 56 périodes où $d = 0,8$ mm, $a = 0,4$ mm et $h = 0,1$ mm. (a) Moule inférieur utilisé pour contenir la poudre à compresser. (b) Moule supérieur utilisé pour compresser la poudre dans le moule inférieur.

La Figure 6.2 (a) présente le moule inférieur servant à contenir la poudre de céramiques. Ce dernier est divisé selon 3 couches. Celle du fond correspond à la cavité destinée à contenir la poudre. La couche du centre, quant à elle, permet de sécuriser le moule supérieur lors de la compression afin de garantir une structure nette. De plus, les dimensions ont été minutieusement choisies afin de permettre à la structure de contenir un prisme de couplage au-dessus de la céramique. Cette configuration, ainsi qu'un système de spectroscopie dans le domaine du temps pour la plage spectrale des térahertz pourra offrir la possibilité de caractériser expérimentalement des modes de surface [81]. Enfin, la couche supérieure présente une structure large, offrant une prise sécuritaire lors du transport du métamatériau. Par la suite, la Figure 6.2 (b) illustre le deuxième moule utilisé pour compresser la poudre. Une fine structure périodique est imprimée afin de pouvoir obtenir, suivant la compression, un métamatériau ayant des paramètres personnalisés d , a et h . Il est à noter que ce dernier, contrairement au premier moule, peut être retiré délicatement une fois la compression complétée.

Une fois la conception terminée, une imprimante 3D peut être utilisée pour fabriquer les moules plastiques. La Figure 6.3 illustre les moules plastiques imprimées à l'aide d'une imprimante 3D Raise3D Pro2 avec une buse d'impression de 0,4 mm. Le filament plastique utilisé est du polypropylène.

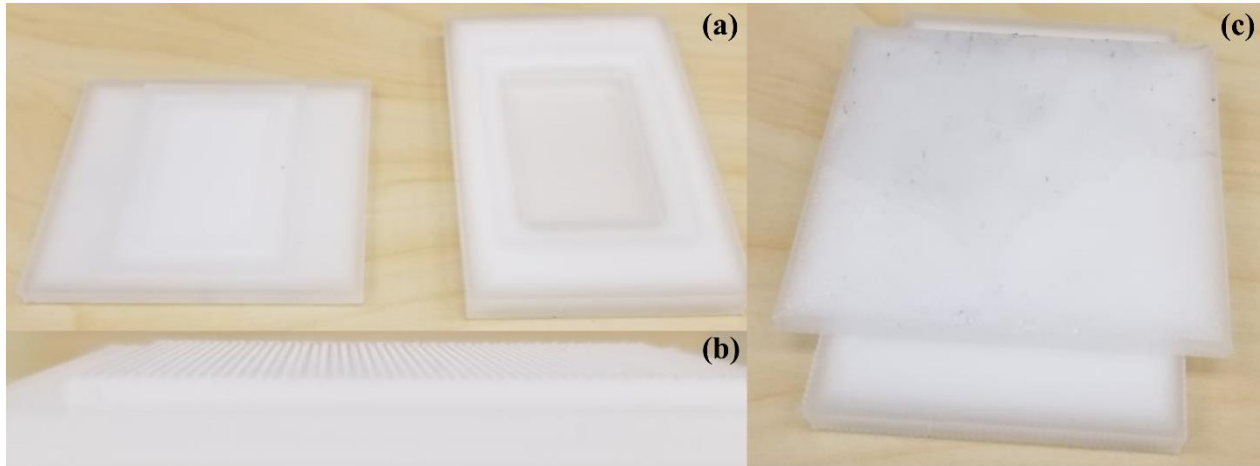


Figure 6.3 (a) Impression 3D des deux modèles à l'aide de l'imprimante Raise3D Pro2 : moule supérieur (gauche) et moule inférieur (droite). (b) Image en gros plan de la fine structure du moule de compression. (c) Assemblage des deux moules plastiques.

6.3 Proposition d'une méthode de caractérisations expérimentales des modes de surface supportés par une surface structurée non conductrice

Pour finir, la structure formée par la compression de poudres de céramiques à l'aide des moules présentés dans la section précédente peut être caractérisée expérimentalement. Plus particulièrement, la partie réelle de la constante de propagation des modes supportés en fonction de la fréquence $\beta_x^{SW,r}(\omega)$ peut être retrouvée à l'aide d'un système de spectroscopie dans le domaine du temps pour le régime spectral des térahertz.

Ce système repose sur la génération et la réception d'impulsion cohérente à larges bandes à l'aide d'antennes photoconductrices, où la détection du champ électrique est obtenue dans le domaine du temps. Cette dernière peut s'obtenir, par exemple, en générant une succession d'impulsions avec un retard temporel croissant τ_0 , où un tel retard est obtenu à l'aide d'une ligne à délai utilisée pour

la modification du parcours optique de la source d'excitation d'une des antennes [158]. Enfin, une transformée de Fourier du signal obtenu dans le domaine du temps est appliquée afin d'obtenir le spectre recherché. Plusieurs domaines d'applications peuvent bénéficier de ce système, telles que l'imagerie térahertz [13], la caractérisation des propriétés optiques de matériaux en fonction de la fréquence (indice de réfraction complexe) [159] et la détection biologique [32, 77]. Ce dernier repose souvent sur l'excitation de modes de surface (modes de résonances) à l'interface entre un métamatériau et une substance à analyser à l'aide d'une source d'excitation directement incidente à la surface, ou encore en utilisant un prisme de couplage placé à proximité de l'interface. Cette configuration, portant le nom d'Otto [83], est employée pour l'excitation de modes de surface et est illustrée à la Figure 6.4.

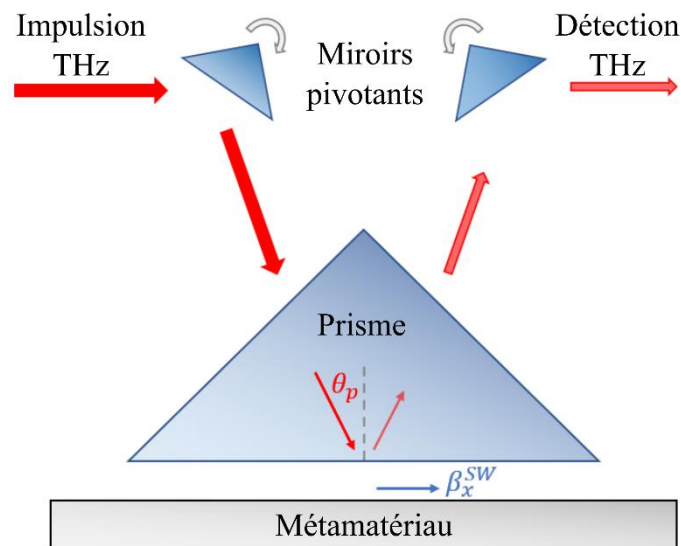


Figure 6.4 Illustration schématique d'un montage en détection basée sur l'excitation de modes de surface à l'aide d'un prisme de couplage ainsi qu'un système de spectroscopie dans le domaine du temps pour la plage fréquentielle des térahertz. L'excitation des modes de résonances à la surface du métamatériau est identifiable à l'aide du spectre de transmission obtenu, où une réduction du coefficient de transmission découle du couplage entre la source d'excitation et le mode de surface. Les miroirs pivotants offrent un contrôle sur l'angle d'incidence θ_p .

Or, la configuration Otto, avec un système de spectroscopie dans le domaine du temps pour la gamme spectrale des térahertz comme source d'excitation et de détection, correspond à une méthode simple et efficace pour l'excitation expérimentale de modes de surface. En effet, telle que

présenté dans le Chapitre 5.8, la condition d'excitation (de couplage entre le prisme et les modes de surface) dépend de l'angle d'incidence de la source d'excitation ainsi que de la fréquence. Expérimentalement, cette condition permet de retrouver la partie réelle de la relation de dispersion $\beta_x^{SW,r}(\omega)$ des modes supportés par le métamatériau non conducteur. Pour ce faire, le spectre de transmission $T(\theta, \omega)$ doit être obtenue en fonction de l'angle d'incidence de la source d'excitation, où la fréquence associée à la valeur minimale de transmission ω_T est reliée à la constante de propagation du mode. Selon la relation de couplage à l'aide d'un prisme (Équation 5.30), cette relation expérimentale prend la forme suivante :

$$\beta_x^{SW,r}(\omega_T) = n_{eff}^{SW}(\theta)k_0(\omega_T) = n_p \sin(\theta_p) \frac{\omega_T}{c} \quad (6.2)$$

où n_p est l'indice de réfraction du prisme de couplage, θ_p est l'angle d'incidence dans le prisme et c est la constante de la vitesse de la lumière. La Figure 6.4 illustre une configuration schématique de cette méthodologie pouvant être appliquée dans un cadre expérimental.

Ce montage pourrait servir à valider le support de modes de surface à l'aide du métamatériau fait de poudres compressées de TiO_2 dans le moule inférieur. Pour ce faire, l'indice de réfraction complexe de la poudre compressée doit d'abord être déterminé expérimentalement afin de connaître la valeur de la permittivité du matériau employé $\varepsilon_m(\omega)$. Le système de spectroscopie dans le domaine du temps peut être employé pour identifier l'atténuation ainsi que le déphasage en fonction de la fréquence d'une impulsion térahertz passant au travers le métamatériau, où l'épaisseur est connue. Ici, l'atténuation et le déphasage de l'onde sont respectivement liées à la partie imaginaire et réelle de l'indice de réfraction de la poudre compressée. Ensuite, une fois ces paramètres connus, un prisme de couplage placé dans le moule (au-dessus de la poudre) est ajouté afin de permettre l'excitation des modes de surface. Enfin, pour plusieurs valeurs de θ_p (angles d'incidences obtenues à l'aide des miroirs pivotants fixés sur des plateformes rotatives à hautes précisions), la relation de dispersion réelle $\beta_x^{SW,r}(\omega_T)$ peut être retrouvée à l'aide des spectres de transmission.

CHAPITRE 7 CONCLUSION

Ce projet de maîtrise a pour mandat l'identification d'une interface capable de supporter des modes de surface dans la gamme spectrale des térahertz (0.1 THz – 10 THz), où les tailles modales ainsi que la distance de propagation sont analogues aux plasmons polaritons de surfaces excitées dans les spectres de l'infrarouge et du visible. Or, cet objectif a été atteint, où une interface alternative composée d'un métamatériau non conducteur est proposée pour le support de modes de surface localisés. Ce dernier se distingue des autres interfaces homogènes révélées lors d'une revue de littérature par sa capacité à fortement localiser l'énergie près de la surface ainsi que dans ces rainures périodiques. De plus, la caractérisation de ce métamatériau révèle une flexibilité importante des propriétés des modes électromagnétiques supportés grâce à ses différents paramètres géométriques, telles que le support de quasi-ondes de surface lentes, rapides et évanescences. Enfin, des méthodes d'excitation ainsi que d'applications potentielles basées sur la détection sont proposées.

Pour caractériser ce nouveau type de métamatériaux pour le support de modes de surface térahertz, une dérivation des équations de Maxwell a été effectuée pour le problème associé à une surface non conductrice présentant des rainures périodiques. Une fois la relation de dispersion analytique obtenue, une caractérisation des propriétés des modes de surface supportés à l'aide de cette structure a été effectuée. Plus particulièrement, les tailles modales ainsi que la distance de propagation théorique de ces quasi-ondes de surface ont été étudiées en fonction des paramètres géométriques, des paramètres optiques ainsi que de la fréquence d'opération. Aussi, afin de valider le développement théorique ainsi que pour obtenir la distribution typique de ces modes électromagnétiques, des résultats numériques, obtenus à l'aide du logiciel COMSOL, accompagnent et confirment les résultats analytiques. Il est à noter que, afin de bien comprendre la nature des modes de surface supportés par ce nouveau métamatériau, l'effort du travail a principalement été sur la compréhension théorique de ces quasi-ondes de surface.

La structure proposée dans le cadre de ce mémoire se distingue des autres métamatériaux discutés dans la littérature pour le support de modes de surface dans le domaine spectral des térahertz par sa composition. En effet, les matériaux hôtes ne sont pas conducteurs et peuvent avoir des constantes de permittivité positive (et même purement positive). Contrairement aux métamatériaux

étudiés par la communauté scientifique qui correspondent majoritairement à des surfaces métalliques structurées, l'interface proposée supporte ainsi un nouveau type de modes de surface, qui se distingue des quasi-ondes plasmoniques qui sont généralement délocalisées dans la gamme spectrale des térahertz. Ces nouveaux modes possèdent des propriétés intéressantes, pouvant mener à l'amélioration dans divers domaines tels que l'imagerie térahertz, la détection biologique ainsi que les guides d'onde compacts. De plus, la possibilité d'opter pour des matériaux alternatifs aux métaux pour le support de modes de surface ouvre de nouvelles opportunités dans la conception de systèmes œuvrant dans la gamme spectrale des térahertz. Cependant, il est à noter que la supposition qu'il n'y a pas d'interaction entre les rainures à travers le matériau lors de la résolution analytique du problème correspond à une limitation. En effet, en réalité, une interaction est attendue à cause de la pénétration du champ dans le matériau. Ainsi, une erreur lors de la détermination expérimentale de la relation de dispersion est attendue. En revanche, pour éviter ces déviations, des absorbeurs entre les rainures pourraient être placés afin d'éviter ces interactions. De plus, opérer dans un régime anti-résonant permettrait d'atténuer l'effet des interactions. Enfin, la relation de dispersion analytique demeure aussi très utile lors de la recherche de solutions numériques sous COMSOL puisqu'elle correspond à un bon point de départ lors de la démarche numérique. Ces solutions, une fois trouvées, peuvent ensuite être utilisées pour la conception de métamatériaux pour des applications pratiques.

Maintenant que la théorie est bien développée, plusieurs nouvelles applications pratiques pourraient être développées à l'aide de ce métamatériau non conducteur. Par exemple, il serait très intéressant de concevoir un détecteur biologique basé sur la résonance de modes de surface et de comparer sa sensibilité avec ceux déjà développés à l'aide de métamatériaux métalliques. Ainsi, en conclusion, la caractérisation rigoureuse de ce nouveau type de métamatériaux pour les domaines œuvrant dans les térahertz sera inciter la conception de nouveaux supports non conducteurs par la communauté scientifique puisque le développement technologique dans cette gamme spectrale est actuellement en ébullition pour son énorme potentiel dans divers domaines d'applications.

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