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Communication

Lattice Resonances in Transdimensional WS_2 Nanoantenna Arrays

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Featured Application: ultra-thin optical components, metasurfaces.

Abstract: Mie resonances in high-refractive-index nanoparticles have been known for a long time but only recently have they became actively explored for control of light in nanostructures, ultra-thin optical components, and metasurfaces. Silicon nanoparticles have been widely studied mainly because of well-established fabrication technology, and other high-index materials remain overlooked. Transition metal dichalcogenides, such as tungsten or molybdenum disulfides and diselenides, are known as van der Waals materials because of the type of force holding material layers together. Transition metal dichalcogenides possess large permittivity values in visible and infrared spectral ranges and, being patterned, can support well-defined Mie resonances. In this *Communication*, we show that a periodic array of tungsten disulfide (WS_2) nanoantennae can be considered to be transdimensional lattice and supports different multipole resonances, which can be controlled by the lattice period. We show that lattice resonances are excited in the proximity to Rayleigh anomaly and have different spectral changes in response to variations of one or another orthogonal period. WS_2 nanoantennae, their clusters, oligomers, and periodic array have the potential to be used in future nanophotonic devices with efficient light control at the nanoscale.

Keywords: transition metal dichalcogenides; Mie resonances; multipole resonances; collective effects; two-dimensional materials; nanomaterials; transdimensional lattices; van der Waals materials

1. Introduction

Nanoparticles and nanoantennae resulting from subwavelength patterning of single- and multi-layer structures have been shown to be an effective way to control light at the nanoscale. High-refractive-index nanoparticles support excitation of multipole Mie resonances of different orders whose strength is mainly defined by the nanoparticle size, index of the material, and ohmic losses. While nanoparticles with moderate refractive index $n \approx 1.45$-2 (e.g., silicon oxide and nitride) have resonances with relatively high radiative losses and low quality factors, materials with $n > 3.5$ (e.g., silicon) enable high mode localization and relatively low radiative losses. Multipole resonances in high-index nanoparticles are comparable to resonances in plasmonic [1] and hyperbolic nanostructures [2,3], as the main role is played by the index difference at the nanoparticle surface.

So far, most of the studies have dealt with silicon [4–8] or III-V nanoantennae [9] because of the readily available fabrication processes and well-established technology. However, recently emerging two-dimensional and layered materials hold great promise to be applied in next-generation optoelectronic devices and more efficient light harvesting [10–12]. Transition metal dichalcogenides (TMDCs), such as tungsten or molybdenum disulfides and diselenides (WS_2, MoS_2, WSe_2, $MoSe_2$) and others, are van der Waals layered materials with high anisotropy, exciton resonances in the visible spectral range, strong nonlinear response, and tunability. Layered material anisotropy results in

different in-plane and out-of-plane permittivity components, and the excitons in visible range result in a large imaginary part of the permittivity along with the increased real part. A large imaginary part not only causes non-radiative losses but also facilities excitation of Zenneck modes and light confinement within the guiding nanolayer [13] or nanoparticles [14]. In the near-infrared range, the losses in TMDCs are near zero, and the nanoparticle can support Mie resonances with high quality factor [15]. Nanoparticle array can be fabricated by patterning TMDC layer (or flakes) using electron-beam exposure of a negative resist and dry etching, see e.g., [15]. An overview of fabrication techniques of transition metal dichalcogenides heterostructure systems can be found in [16].

Nanoparticle resonances can be enhanced, and their spectral position can be controlled not only by the nanoparticle size, shape, and material but also their arrangement in the clusters and/or lattices [17–24]. Nanoparticle clusters facilitate excitation of narrow Fano resonances [1] that are very sensitive to the parameter changes, can be easily tuned in the spectral domain or lost because of the imperfections. In contrast, the periodical arrangement of nanoparticles in the lattice enables excitation of lattice resonances that have a relatively high tolerance to local imperfections. The spectral position of different multipoles can be controlled by mutually perpendicular periods of the nanoparticle array [25,26].

In this work, we report on the theoretical prediction of Mie resonances in a periodic array of WS_2 nanodisks and their control by the lattice dimensions. We show excitation of multipole resonances in the proximity to the Rayleigh anomaly λ_{RA} (wavelength equal to the product of surrounding refractive index n and array period $p_{x,y}$, $\lambda_{RA} = np_{x,y}$) and a different optical response depending on the period changes in such a transdimensional lattice. The lattice resonances can be observed as a peak in reflection and absorption at the wavelength $\lambda \approx \lambda_{RA} = np_{x,y}$. Because of the high real part of WS_2 in-plane permittivity tensor component in the near-infrared range, the lattice resonance of the electric dipole is excited even for large and elongated periodic cells (240×700 nm^2).

2. Results

We consider a periodic rectangular array of WS_2 nanodisks surrounded by a uniform medium with moderate refractive index $n = 1.5$ (equivalent to matched-index substrate and superstrate, Figure 1a). Permittivity components of WS_2 are presented in Figure 1b where $\varepsilon_{||}$ is in-plane and ε_{zz} is out-of-plane tensor components and $\varepsilon_{WS2} = (\varepsilon_{||}, \varepsilon_{||}, \varepsilon_{zz})$. One can see that losses of $\varepsilon_{||}$ are relatively high for $\lambda < \lambda_c = 655$ nm, and nanoparticle resonances in this spectral region are not well defined for a dense array. At the same time, for $\lambda > \lambda_c$, the absorption peak is clearly seen for the electric dipole (ED) resonance $\lambda_{ED} \approx 697$ nm (Figure 1c, red line and Figure 1d), which indicates excitation of Mie resonance. The E-field profile at $\lambda = 697$ nm in Figure 1d is not the one of a pure ED multipole but the distribution is clearly seen with the main contribution of ED resonance. Absorption is calculated as losses in the nanoparticle regardless of the number of diffraction orders taken into account, and the resonance is associated with an increase in reflection at the wavelength about 690 nm (Figure 1c, blue line).

We analyze the absorption and reflection properties in the transdimensional lattice [27] with different periods in orthogonal direction p_x and p_y. In numerical modeling, we consider the normal incidence of light, one WS_2 nanodisk in the unit cell, periodic boundary conditions in x- and y-directions, and the artificial perfectly matched layers in the z-direction. We perform numerical simulations with finite element method implemented in CST Microwave Studio frequency-domain solver.

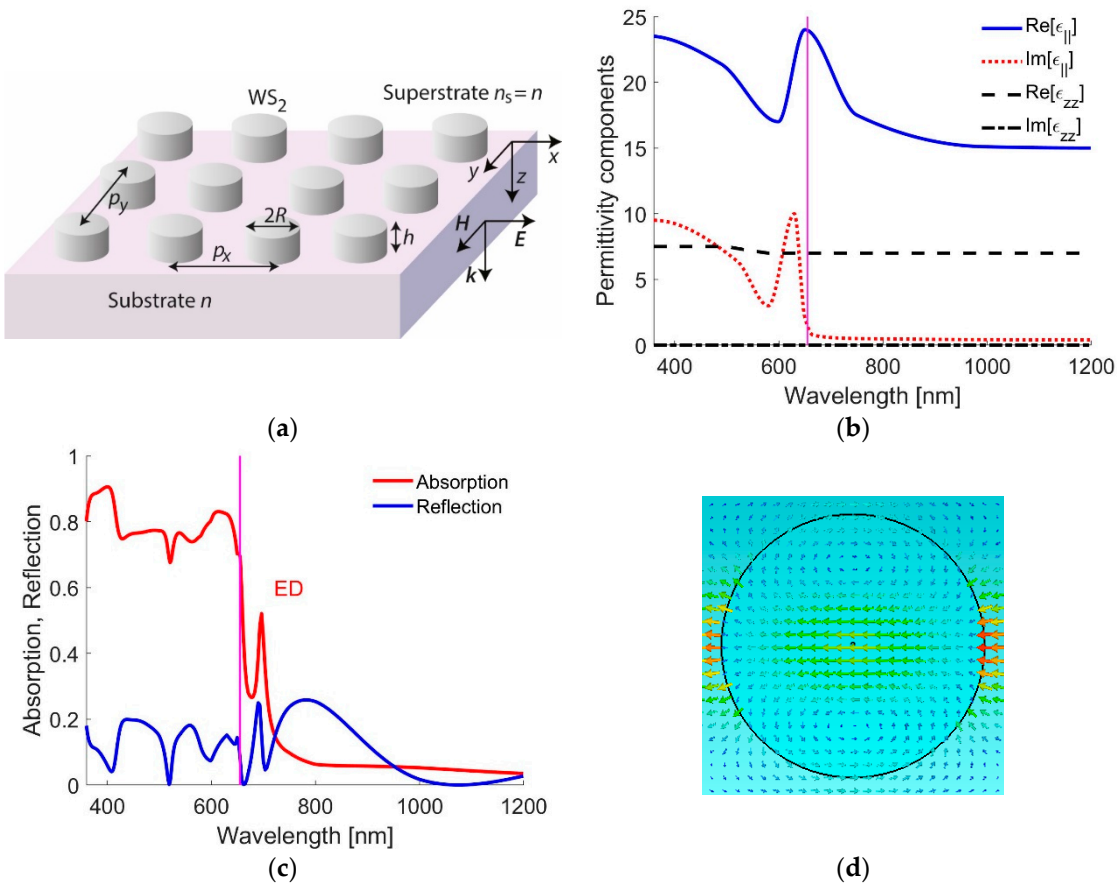

Figure 1. (**a**) Schematic of the transdimensional lattice under consideration. The parameters are the following: nanodisk radius R = 100 nm, height h = 200 nm, and refractive index of surrounding $n = n_s$ = 1.5. (**b**) WS_2 permittivity components. (**c**) Absorption and reflection from the nanoparticle array with periods $p_x = p_y$ = 240 nm. Magenta lines on (b) and (c) panels indicate the wavelength λ_c where WS_2 absorption drops significantly, and for $\lambda > \lambda_c$, the nanoparticles support Mie and lattice resonances. (**d**) E-field distribution at λ = 697 nm indicating ED contribution of the resonance.

For a spherical particle with isotropic constituent material, each of these periods controls different lattice resonances: under illumination with x-polarized light, p_x controls the magnetic dipole (MD) and electric quadrupole (EQ) resonances, and p_y controls ED and magnetic quadrupole (MQ) [17,24,25]. These considerations are approximately valid for disks even though the description of the particle includes a tensorial polarizability. Calculations in Figure 2 show that under change of p_y, the ED resonance shifts to longer wavelength. In Figure 2, calculation results are terminated at Rayleigh anomaly wavelength $\lambda_{RA} = np_{x,y}$ to account for only sub-diffraction effects. Upon further increase in the period (p_y > 400 nm), the ED transforms to ED-lattice-resonance (ED-LR) and follows the Rayleigh anomaly. Even for fairly large periods p_y > 700 nm, the resonance is well defined, and one can see peaks in absorption and reflection profiles. Similar to the effect of p_y changes, changes in p_x result in the excitation of lattice resonances in the proximity to the Rayleigh anomaly, but the resonances do not extend to a longer wavelength. This behavior is typical for the nanoparticles with rapidly decreasing polarizability.

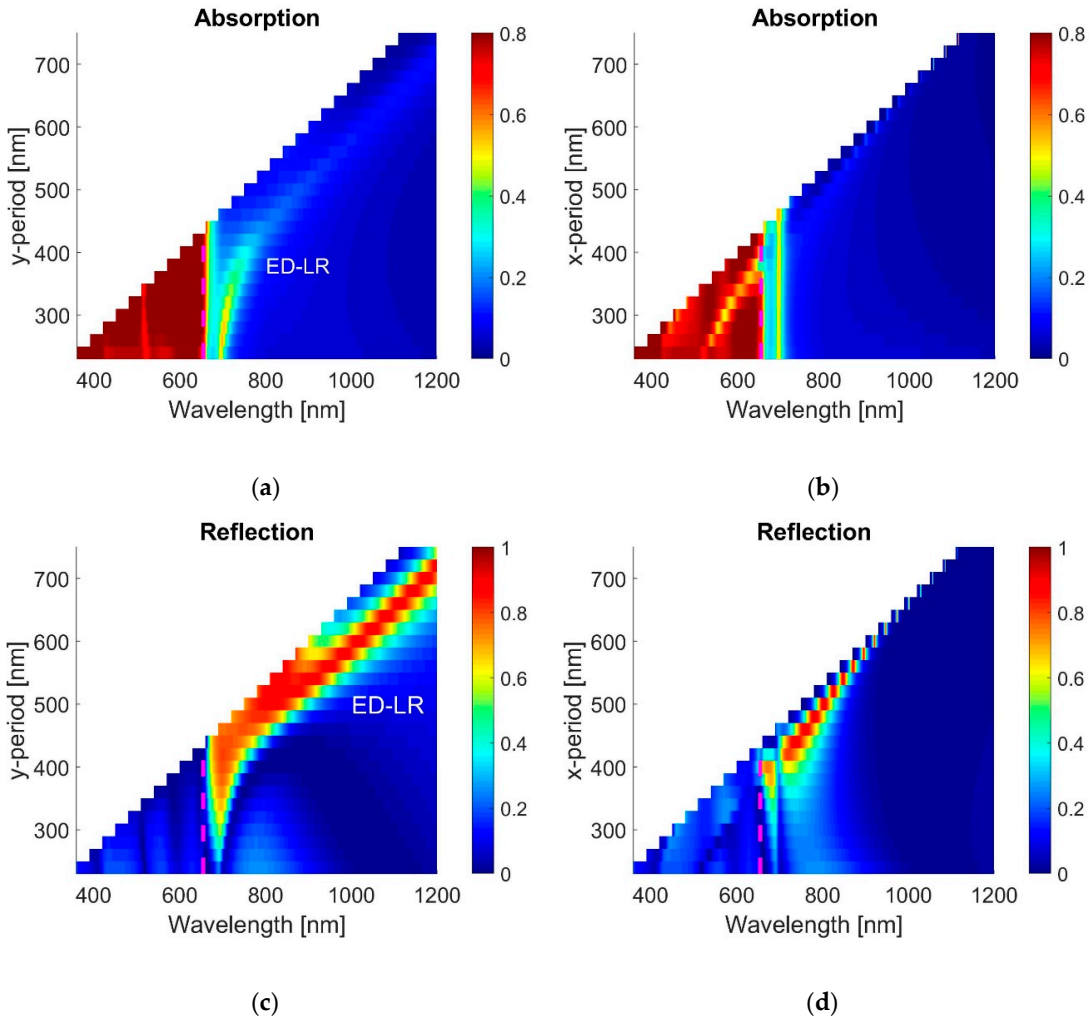

Figure 2. (**a**,**b**) Absorption and (**c**,**d**) reflection in nanoparticle array for different periods. In (**a**,**c**) period p_y changes and p_x = 240 nm. In (**b**,**d**), period p_x is changes and p_y = 240 nm. Magenta dashed lines indicate the same wavelength of absorption drop λ_c as in Figure 1. Electric dipole lattice resonances (ED-LRs) appear for a change of the period p_y, which is in full agreement with the analytical considerations for incident field **E** along the x-axis. Calculation results are terminated at Rayleigh anomaly wavelength $\lambda_{RA} = np_{x,y}$ to account for only sub-diffraction effects.

3. Conclusions

To sum up, we have studied a transdimensional lattice consisting of a two-dimensional periodic arrangement of WS_2 nanodisks with single-particle Mie resonances defined by disk parameters in all three dimensions. Even though the TMDC family of materials have high permittivity comparable to silicon and III-V materials, the idea of engineering Mie resonances in nanoparticle lattices and designing metasurfaces based on them remain overlooked. In this work, we show that well-defined Mie resonances are not only excited in single or closely packed nanodisks but the resonances can be also shifted by the array periods. Because of the high value of in-plane permittivity component in the visible and near-infrared spectral ranges, the lattice resonances of the electric dipole can be excited even in the elongated lattice and in a broad spectral range.

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