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Numerical investigation of nonlinear photothermal effect in Vanadium Dioxide phase-change particles

Binhe Wu [a,*], Min Zhao [a], Jian Zhou [b], Xiaofeng Xu [a], Chunrui Wang [a]

[a] Department of Applied Physics, Donghua University, No. 2999, North Renmin Road, Songjiang District, Shanghai 201620, China
[b] Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, No. 865, Changning Road, Shanghai, 200050, China

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ABSTRACT

Modulating the material temperature as well as its optical response promises various potential applications of photothermal effects. In this work, we develop a self-consistent simulation scheme to investigate the nonlinear photothermal response of Vanadium Dioxide (VO_2) particles where the material can be driven from insulating to semiconducting phases or vice versa. Our results indicate that the photothermal-induced phase change process can be an efficient degree of freedom in designing micro- or nanoscale structures for photothermal applications. Moreover, for particle dimers, the particle temperature can be tuned by varying the particle distance and the polarization of the incident light. Our findings then suggest the possibility for designing and optimizing particle dimers to characterize the light polarization by measuring dimer temperature.

1. Introduction

Engineering the thermal and optical responses of metallic or dielectric particles via photothermal effect [1] has been the subject of much interest in recent studies [2–5]. Particles under light illumination has enabled potential applications such as photothermal therapy [6,7], photothermal imaging [8,9], vapor generation [10,11], hot printing [12] and light-assisted material growth [13–15]. The main mechanism underlying these applications are the tunable particle temperature due to heat deposition in materials under light illumination. A fact which has attracted less attention is the sensitivity of the heat generation to the variation of the material optical properties which in turn depend on the temperature change [16]. Careful tuning the material properties via photothermal effect can thus provide an additional degree of freedom in designing novel functionalities. For example, experiments have shown that when material particles are immersed in fluids, the surrounding refractive index can be modified due to the photothermal effect. The effect can equivalently act as a thermal lens. As a result, a quantitative measurement of the temperature distribution has been enabled by mapping the wavefront distortion of the optical wavefront crossing the system [17,18]. However, the resolution as well as the precision of this temperature measurement remains limited in reality as the local refractive index variation is quite weak for moderate temperature increase. To make better use of this tunable photothermal response, it would be advantageous to magnify the variations of material properties at moderate light absorption.

Phase change processes are one of the most complicated aspect of thermodynamics which may drastically modify the material optical properties over a wide spectrum. It is thus interesting to investigate how the thermally induced phase change processes can be correlated to the photothermal effect. This correlation enables us to develop tunable broadband optical modulators or switches by tuning the frequency or intensity of the incident light.

In this study, we take the Vanadium dioxide (VO_2) particles as such a model material and investigate its nonlinear photothermal effect correlated with the phase change processes. VO_2 has been known as a versatile phase-change material for over five decades [19,20]. It can undergo a reversible insulator to semiconductor phase transition around the critical temperature of 68 °C. Experiments have shown that the phase change can be triggered by several means such as the temperature, electric field, light excitation or strain. Along with the phase change process, the optical properties of VO_2 can be dramatically changed in the infrared and terahertz spectrum. This has enabled us to develop the highly desired broadband and high-modulation-depth devices working in the far infrared and terahertz region [21,22]. However, an accurate analysis of the correlation of photothermal effect and optical response of the phase change material remain less investigated in previous studies. Such theoretical study demands numerical frameworks coupling electromagnetic simulation and the thermal dynamics as the light absorption and heat dissipation are competing mechanisms that govern the actual temperature as well as the phase and material properties

* Corresponding author.
E-mail address: bhwu@dhu.edu.cn (B. Wu).

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in the system. In recent studies, Yu et al. [23] solved the coupled light absorption and heat diffusion in metallic nanoparticles with the method of moments. However, the variation of material properties to the temperature change is not taken into account. We have previously developed a self-consistent numerical simulation scheme to take into account the electromagnetic wave propagation and heat dissipation in VO_2 films with gold gratings [24]. The electromagnetic wave is simulated using the rigorous couple wave analysis (RCWA) method and the heat dissipation accounts the conduction loss. Our numerical results show that the material properties can be tuned by the nontrivial coupling of the plasmonics of Au gratings and the thermal transport in the VO_2 films. As a result, an active grating can be realized by tuning the external light field. However, the simulation scheme becomes invalid for many applications of the photothermal effect where the objects are immersed in fluids. These situations lack structural periodicity and the main mechanism for heat dissipation can be the heat convection.

The main object of the present work is thus to develop a coupled electromagnetic and thermal simulation scheme for photothermal effect. We then apply the simulation approach to study quantitatively and self-consistently the influence of a continuous wave illumination on the optical as well as thermal response of VO_2 particles floating in the air. Generally, the most time consuming part in the simulation is solving the Maxwell's equation. Diverse analytical or numerical methods [25,26] such as the Mie theory, the Finite-Difference Time-Domain method, the Finite-Difference Frequency Domain method, and the methods based on integral equations are developed to obtain the light absorption. In this study, we numerically simulate the electromagnetic waves through the particles with the volume integral equation (VIE) method [27] which can numerically give direct results of the optical scattering and heat generation in objects with arbitrary geometries. In our device, the heat deposition in the particle can increase its temperature and be dissipated by the convection to the environment. Our results show that the nonlinear photothermal effect due to phase change processes can drastically amplify the variation of material properties. It enables various potential applications such as modulation, switching and microscale temperature mapping. Our numerical results also show that the photothermal effect can be enhanced in two closely coupled particles. The enhancement is sensitive to the interparticle distance and the polarization of the incident light respect to the alignment of the double particles.

The rest of the paper is organized as follows. In Section 2, we introduce the model system, the formulas and the numerical scheme to simulate the nonlinear photothermal effect. In Section 3, the numerical results and their discussions are presented. Finally, a conclusion is given in Section 4.

2. Theoretical formalism

As model system, we study VO_2 spherical particles under light illumination. The radius of the particles is R. The particles are illuminated in steady state by an external monochromatic plane wave radiation of wavelength λ and light intensity I_{inc}. Heat is generated in the particles due to light absorption. Heat transfer between the particle and its environment is assumed to be dominated by natural convection. The environment temperature is T_∞. To self-consistently determine the photothermal response of the particles, the first step is a solution to the Maxwell equations to characterize the optical absorption. In this study, we apply the VIE method [27] to simulate the light scattering in the particles. For non-magnetic objects with arbitrary dielectric profile, the VIE can be written as

$$\vec{E}_{\text{inc}}(\vec{r}) = \frac{\vec{D}(\vec{r})}{\varepsilon(\vec{r})} - (k_0^2 + \nabla\nabla\cdot)\vec{A}(\vec{r}) \tag{1}$$

where $k_0^2 = \omega^2(\varepsilon_0\mu_0)$ and ω is the frequency, $\vec{E}_{\text{inc}}$ is the incident electric field of light, $\varepsilon(\vec{r})$ and ε_0 are, respectively, the permittivity profile of the inhomogeneous materials and vacuum, $\vec{D}$ is the electric flux density and $\vec{A}$ is the vector potential which is given by

$$\vec{A}(\vec{r}) = \frac{1}{\varepsilon_0}\int G(\vec{r}-\vec{r}')\chi(\vec{r}')\vec{D}(\vec{r}')d\vec{r}'.$$

Here $G(\vec{r}) = \frac{\exp(ik_0r)}{4\pi r}$ is the Green's function and χ represents the normalized contrast function which is defined as

$$\chi(\vec{r}) = \frac{1}{\varepsilon(\vec{r})}(\varepsilon(\vec{r}) - \varepsilon_0).$$

In Eq. (1), the first term on the right hand side (RHS) represents the exact electric field distribution in the simulating domain while the second term is the scattering electric field which fulfills the boundary conditions. Their difference characterizes the incident electric field. In numerical simulation, we employ the cuboid cells to discretize the simulating domain where the cubic volume is $\Delta V = \Delta x\Delta y\Delta z$ and Δx, Δy, Δz are, respectively, the grid sizes along x, y and z directions. Furthermore, the physics functions such as $\vec{D}$, $\vec{A}$ and $\vec{E}$ are expanded using the rooftop basis functions [25]. As a result, the discrete form for the vector potential is given by

$$A^{(u)}_{M,N,P} = \Delta V \cdot \sum_{M',N',P'} G_{M-M',N-N',P-P'}\chi^{(u)}_{M',N',P'}d^{(u)}_{M',N',P'} \tag{2}$$

where u stands for either x, y, or z and $\vec{d} = \vec{D}/\varepsilon_0$. To eliminate possible singularities, the function values at discrete grids are evaluated via the spherical mean method [27]. In evaluating Eq. (2), a three-dimensional fast Fourier transform is efficient in the computations of the discrete convolutions. Finally, the linear equations arising from the discrete form of Eq. (1) can be solved by the Stabilized Bi-Conjugate Gradient iterative method (BiCGSTAB) [28] to arrive at the exact field distribution $\vec{E}(\vec{r})$ in the simulation domain. Good agreement of our numerical simulation with the existing results [27] as well as the prediction of Mie theory is achieved.

After solving the electric field, the absorbed power density in the particle can be evaluated by

$$p(\vec{r}) = \frac{\omega}{2}\text{Im}\left(\varepsilon(\vec{r})\right)|\vec{E}(\vec{r})|^2,$$

where Im stands for the imaginary part. The total absorbed power can be evaluated by integrating the absorbed power density in the volume

$$P_{\text{abs}} = \int p(\vec{r})d\vec{r}.$$

The heat deposited in the spherical particle can be characterized by the absorption efficiency Q_{abs} which is defined as

$$Q_{\text{abs}} = \frac{P_{\text{abs}}}{I_{\text{inc}}S_0}, \tag{3}$$

where $S_0 = \pi R^2$. I_{inc} is related to the incident electric field $\vec{E}_{\text{inc}}$ as

$$I_{\text{inc}} = \frac{\varepsilon_0 c}{2}|\vec{E}_{\text{inc}}|^2,$$

where c is the speed of light.

Although the absorption power density could be markedly non-uniform, the resulting temperature distribution in the particles with moderate size can be taken as uniform due to the large difference between the thermal conductivities of the particle and the surrounding gas. We can therefore for the sake of simplicity assume an uniform temperature across the particle.

Normally, the generated heat due to light absorption in the particles can be transferred to the surrounding media via either conduction, convection or radiation. Most of previous studies have taken the conduction to be the main heat dissipation mechanism in photothermal effect, while convection and radiation is less investigated. We note in a recent study, Kallel et al. [29] numerically studied the temperature of gold nanoparticles above an substrate where the only heat dissipation is via the radiative heat loss from the particle to the environment. For the present situation where the particle is immersed in air, the main mechanism for heat dissipation is the natural convection since the conduction is less efficient in air and the thermal radiation is quite weak at low temperature differences [30]. Without diving into the details of thermal and fluid dynamics, we obtain the rate of heat transfer by natural convection from a solid surface at a uniform temperature T to