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Pressure dependency of electron-phonon renormalization in diamond

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ABSTRACT

Employing ab initio many-body perturbation theory, the carrier-phonon and carrier-carrier vertex functions are evaluated in diamond crystal under different hydrostatic pressure up to 140 GPa and the phonon induced quasiparticle renormalization is measured at diverse linear and non-linear pressure regimes. Our results illustrate that the degree of carrier coupling to phonon satellite differs substantially from linear to non-linear regimes, due to changing the nature of the carrier dynamics. Particularly, reduction of the phonon induced renormalization with increasing pressure on the system is an indication of a transition from strong to a weak polaronic nature, which is in good accordance with experimental and theoretical studies. It demonstrates the significant role of the pressure in tuning the electron phonon coupling in a system. Furthermore, going to the higher pressure yields relevant discrepancy in electron energies from second-order phonon-induced to the first-order phonon perturbation. Our study recommends the hydrostatic pressure adjusts the significant contribution of electron-phonon self-energy in the electronic-related features of carbon-based materials as a new probe.

1. Introduction

A thorough understanding of the physical origins of unique carbon-based material properties at high pressures is still far from being achieved. Diamond as a famous 3D tetrahedrally bonded insulator under high hydrostatic and non-hydrostatic pressures has attracted much attention due to its extreme hardness [1]. One of the profound and challenging effects which plays a major role, is electron-phonon coupling which elastic or inelastic kind of carrier scattering from phonons as well as the energy exchange is the relevant part of carrier dynamics [2,3]. Hot carrier dynamic is important for device speed controlling and also time-resolved interpretation of excited states [4,5]. On the other hand, one can engineer the electronic properties of materials via applying hydrostatic pressure because deformation potential changes the chemical bond, shape of band structure, phonon frequency and even the crystal structure [6]. Therefore, understanding the mechanism of hot carrier thermalization under high hydrostatic pressures has sparked many opportunities to be exploited in the broad range of technological importance.

There are theoretical works, which address the strength of electron-phonon (el-ph) coupling in diamond. From frozen-phonon approach [7,8], DFPT method with direct computation of el-ph in the migdal framework [3,9,10], Monte carlo calculation [11,12] to molecular dynamics calculation [13], all indicate sizable value for el-ph renormalization as a result of the considerable coupling of optical mode to electronic degree of freedom and the presence of self-trapping due to the formation of nearly large polaron.

On the other hand, in the context of electron relaxation, the second important scattering mechanism is electron-electron correlation far away from band edges. One study [14] based on many body perturbation calculation of electron self-energy in GW method, shows the Fermi liquid behavior of electronic lifetime with emphasis on the important role of plasmon in thermalization of electrons. Other recent studies [15,16] also imply the important interplay effect of electron-electron correlation on the temperature dependence of band structures arising from electron-phonon coupling.

Besides, there are several studies, which address application of high compressive hydrostatic pressure on diamond crystal [17,18]. Occelli et al. [19] have studied the stability of diamond properties under hydrostatic pressure up to 140 GPa and obtain diamond treats as a Gruneisen solid so that optical phonon frequency shifts can be used as a useful gauge in the non-linear multi-megabar pressure effect range. Another study indicates that the application of high hydrostatic pressure enhances the thermal conductivity of diamond crystal [20]. The reason is an overall increased frequency shift that yields larger acoustic velocities, which makes the reduction of phonon-phonon scattering. Other available works [21,22] show non

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linearity of pressure in terms of phonon frequency. Moreover, it was shown that the thermal conductivity is influenced by volumetric electron-phonon coupling along with phonon-phonon thermalization in metal-diamond contact at high-pressure [23]. All the abovementioned findings suffer from the lack of direct understanding of the interplay between applying pressure and the degree of electronic to lattice coupling. Therefore, controlling the thermalization of the carrier by engineering of electronic structure in the presence of high nonlinear pressure regime is of great importance. Having earned the matrix elements of the carrier-phonon and carrier-carrier interaction, the relationship between the carrier velocity renormalization and external pressure can be extracted in both linear and nonlinear pressure-volume regimes. Present work opens a way toward understanding of mutual behavior between carrier-phonon scattering as well as carrier-carrier scattering and hydrostatic pressure, which entirely be utilized for designing novel tailored technological devices. The paper is organized as follows. In Section 2, we describe the computational details used for computing the electron-phonon coupling matrix elements. In Section 3 our results of pressure dependency of electron-electron along with electron-phonon scattering rates are presented. Finally, we discuss our findings in Section 4.

2. Computational method

Hydrostatic compressive pressure was applied on diamond crystal in 0, 40, 80, 120 and 140 GPa which results in changes in bonding, elasticity and also electronic excitations. Here, we are interested in the calculation of the effect of hydrostatic pressure on the rates of electron thermalization via scattering from other electrons and phonons.

Many body approach [5,24,25] gives thermalization rate of an excited electron falling into the conduction band with the rest of electrons across the valence band by the imaginary part of electronic self-energy:

$$\tau^{-1} = -2\int dr \int dr\phi_i'(r) Im\Sigma_{el-el}(r, r'; \epsilon_i)\phi_i(r') \tag{1}$$

where ϕ_i and ϵ_i is electron orbital and electron energy, respectively. The self-energy is written based on Hedin formalism [24] as:

$$\Sigma_{el-el}(r, r' : \epsilon_i) = \frac{i}{2\pi}\int d\epsilon_i' e^{-i\delta^+\epsilon_i'} G(r, r' : \epsilon_i' - \epsilon_i) W(r, r' : \epsilon_i') \tag{2}$$

which within the GW approximation, G is the Greens function of the electrons, and W is the dynamically screened Coulomb interaction and δ^+ is a positive infinitesimal time. Dynamical screened correlation within plasmon pole approximation as implemented in Yambo code [26] was used in our calculation. We consider total number of 100 bands and k-point mesh of $8 \times 8 \times 8$ were included to reach converged value of quasiparticle energy and have well converged rates for diamond crystal under each individual pressure, respectively.

Density functional perturbation theory [27] are exploited to compute the dynamical lattice features including phonon dispersion and deformation potentials under applying abovementioned hydrostatic pressures. Then, the el-ph self-energy Σ^{el-ph} for electron dynamical behavior within the energy band n and wavevector k in first-BZ are founded employing EPW code [28] which $Im\Sigma_{nk}^{el-ph}$ due to the el-ph coupling contribution within Migdal approximation [9] is represented as:

$$Im\Sigma_{nk}^{el-ph} = \sum_{nm,k}^{\lambda,q} |W_{nm,k}^{\lambda,q}|^2 Im\left\{\frac{N_{\lambda,q} + f_{m,k} + 1}{\epsilon_{n,k} - \epsilon_{m,k+q} - \hbar\omega_{\lambda,q} - i\delta} + \frac{N_{\lambda,q} - f_{m,k}}{\epsilon_{n,k} - \epsilon_{m,k+q} + \hbar\omega_{\lambda,q} - i\delta}\right\} \tag{3}$$

where N and f are Bose and Fermi-Dirac occupations, $\hbar\omega_{\lambda,q}$ is energy of phonon with polarization of λ in the wave-vector of q and η is a small smearing quantity. Fundamental term includes el-ph matrix informations are written as:

$$W_{nm,k}^{\lambda,q} = \left\langle \Phi_{m,k+q} | \frac{\partial U_{scf}}{\partial u_{q,\lambda}} | \Phi_{n,k} \right\rangle \tag{4}$$

where $\Phi_{n,k}$ is KS orbital and $\frac{\partial U_{scf}}{\partial u_{q,\lambda}}$ is the derivative of self-consistent potential for an ion moving along mode in λ branch and q wavevector. The el-ph matrix electronic and vibrational states are calculated on finer mesh of $40 \times 40 \times 40$ k and q points with sufficient interpolation based on Wannier orbitals as used in EPW code [28]. Wannierization is performed taking 4 valence and 4 conduction bands with hybrid sp^3 orbitals exactly on C atoms.

Our primary DFT results are performed using norm-conserving pseudopotential within local density approximation LDA exchange-correlation functional was formulated in Perdew-Zunger [29] scheme available in QUANTUM ESPRESSO package [30]. Equilibrium lattice parameter is 3.514 Å with an energy cutoff of 60 Ryd for plane-wave basis set integration and a mesh of $(12 \times 12 \times 12)$ k-points for Brillouin zone integration for all pressure values.

3. Results and discussion

3.1. Pressure dependency of diamond volume

Since applying hydrostatic pressure crucially changes electronic band structure and also phonon dispersion, it is advantageous to measure the order of coupling between electronic and lattice degree of freedom. One of the common effects that can probe this interplay is phonon frequency shift induced by the change of volume for an arbitrary strain which can be represented as Gruneisen parameter as $\gamma = -dln\omega/dlnV$. Normally, the Gruneisen parameter varies from 0.5 to 3 for typical covalent crystals and crystals with van der Waals nature [31], thereby it can reflect the degree of anharmonicity.

It is argued that Gruneisen parameter can be decomposed into two contributions, the first is due to direct phonon-phonon interaction and the second is due to the indirect phonon-phonon interactions via coupling with charge carriers [32] (measuring electron-phonon coupling). By the exertion of the pressure, we are able to tune the second part of Gruneisen term i.e. el-ph scattering and thereby, control the thermodynamic properties.

Here, we address the pressure dependence of diamond volume from 0 to 140 GPa as shown in Fig. 1. Our computational data for v(p) are consistent with available experimental data were done by X-ray diffraction and are fitted by Vinet equation of state [19,33]. Clearly, the nonlinear pressure regime starts from nearly 100 GPa consistent with experimental data of diamond anvil cell measurement [19]. Moreover, the pressure-phonon frequency relationship $\omega(p)$ at degenerate Γ point, recovers linear dependence near ambient pressures and quadratic dependence at higher pressures, consistent with previous experiment and theoretical results [19,34]. Around 100 GPa, the transition from linear to nonlinear behavior which also is accompanied by linear to the nonlinear treatment of Raman frequency of optical mode versus applied pressure, is attributed to the increase in the covalent type nature of diamond. On the other hand, the enhancement of covalent bonding under compressive hydrostatic pressure which doesn't alter the cubic crystal symmetry, results in opening the band gap by increasing the band-width as a result of uniform reduction in the atomic distances. Therefore, above-mentioned changes in the electronic structure and phonon dispersion yield the significant variations in the strength and nature of the coupling between electron and phonon channels, particularly starts around 100 GPa. Hence, it seems that the below and above