

First Principles Calculation of Electron-Phonon Scattering Rates in Si

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Abstract

A first principles LDA approach based on the Harris functional ansatz is used to investigate the electron-phonon interaction in silicon, within the rigid ion approximation. Electron-phonon matrix elements for transitions between selected electronic states are calculated, and used to generate band- and wavevector-dependent scattering rates. These scattering rates are generally larger than those calculated with other methods, and show significant anisotropy.

I. Introduction

The concept of applying pseudopotentials to the analysis of electron-phonon interactions in solids [1] has served as an invaluable tool in our theoretical understanding of the process. Without pseudopotentials, one currently either relies on a restricted scope of measurable information, or is relegated to phenomenology. Primarily for purposes of simplicity, most investigations of the electron-phonon interaction in semiconductors have made use of empirical pseudopotentials [2-6], mostly in the local approximation [2-5]. As the true crystalline pseudopotential is necessarily nonlocal, some authors have added correction terms [5,6]. While useful in gaining insight, these empirical approaches suffer from their sensitivity to several adjustable parameters as some authors have noted [5, 7]. For example, before any electron-phonon analysis takes place, all of the local form factors must be treated as free parameters and adjusted such that the resulting bandstructure matches experimental values at a suitably defined set of points in the Brillouin zone [8]. Additionally, due to the nature of the electron-phonon interaction potential, one must still choose among various interpolation and extrapolation schemes between and beyond these discrete adjustable form factors in reciprocal space. Of particular concern is the finding that the most physically meaningful choice of extrapolation criteria do not yield the best results [5]. For these and other reasons, several authors have chosen an alternative approach.

It has long been known [9] that electron-phonon matrix elements calculated using pseudopotentials can in principle be just as accurate as those calculated using the true potential, as long as the pseudopotentials are calculated directly from the true potential. This has led to several *ab initio* investigations based on density functional theory [10, 11, 12] in the local density approximation (LDA). Such self-consistent Kohn-Sham (K-S) type calculations quite naturally avoid all of the difficulties of the empirical approach mentioned above. Furthermore, the self-consistent LDA calculations implicitly include the effects of atomic polarization, which is impossible to include using the empirical pseudopotentials.

With all of these benefits, the K-S method has the drawback that modern computational resources limit its application to a small set of high-symmetry transitions due to the requirement of self-consistency.

An alternative approach [7] which uses the *ab initio* pseudopotentials yet avoids the problem of self-consistency involves an approximation to the change in crystalline charge density when the atoms are displaced. This approximation, based on the Harris functional ansatz [13], is to replace the self-consistent K-S potential with one derived from overlapping atomic charge densities. The benefit of this approach is the flexibility to calculate electron-phonon matrix elements for arbitrary transitions, yet it remains a first-principles theory. In the following sections, the method is briefly described, and then used to generate band- and wavevector-dependent scattering rates for silicon.

II. The Model

One may write a crystalline density functional non-interacting Hamiltonian using pseudopotentials as

$$H = -\frac{1}{2}\nabla^2 + \sum_l \Delta V_{ps,nl}^l(\mathbf{r}, \mathbf{r}') + V_{ps,loc}(\mathbf{r}) + V_H[n(\mathbf{r})] + V_{ex}[n(\mathbf{r})] + V_{co}[n(\mathbf{r})], \quad (1)$$

where $V_{ps,loc}(\mathbf{r})$ is the local crystalline ionic pseudopotential, $\Delta V_{ps,nl}^l(\mathbf{r}, \mathbf{r}')$ is the nonlocal l -dependent ionic crystalline pseudopotential, and $V_H[n(\mathbf{r})]$ is the Hartree potential. $V_{ex}[n(\mathbf{r})]$ and $V_{co}[n(\mathbf{r})]$ are functional derivatives of the exchange and correlation energies with respect to pseudocharge density. Single electron wavefunctions are expanded in a plane wave basis as

$$\Psi_{\mathbf{k},n}(\mathbf{r}) = \frac{1}{\sqrt{N\Omega_0}} \sum_{\mathbf{G}} Z_{\mathbf{k},n}(\mathbf{G}) e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}}, \quad (2)$$

and matrix elements of this pseudopotential Hamiltonian are taken with respect to these basis functions leading to the familiar secular equation

$$\det \left| \left(\frac{1}{2}(\mathbf{k} + \mathbf{G}')^2 - E_{\mathbf{k},n} \right) \delta_{\mathbf{G}',\mathbf{G}} + V_{ps,tot}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}') \right| = 0 \quad (3)$$

which defines the eigen-energies and wavefunctions.

As is usual, the bare ionic potential (nucleus with core electrons) is expanded in a series under the assumption of small displacements,

$$V_b(\mathbf{r}) = \sum_{j,\alpha} [V_b(\mathbf{r} - \mathbf{R}_j - \tau_\alpha) + \delta\mathbf{R}_{j,\alpha} \cdot \nabla V_b^\alpha(\mathbf{r} - \mathbf{R}_j - \tau_\alpha) + \dots], \quad (4)$$

ignoring multi-phonon processes [14] and any polarization of the bare ions themselves under displacement. Since the first order term is much smaller than the zero order term, the electron-phonon interaction is treated perturbatively, with the screened first order term giving rise to transitions between eigenstates of the screened zero order term. In the

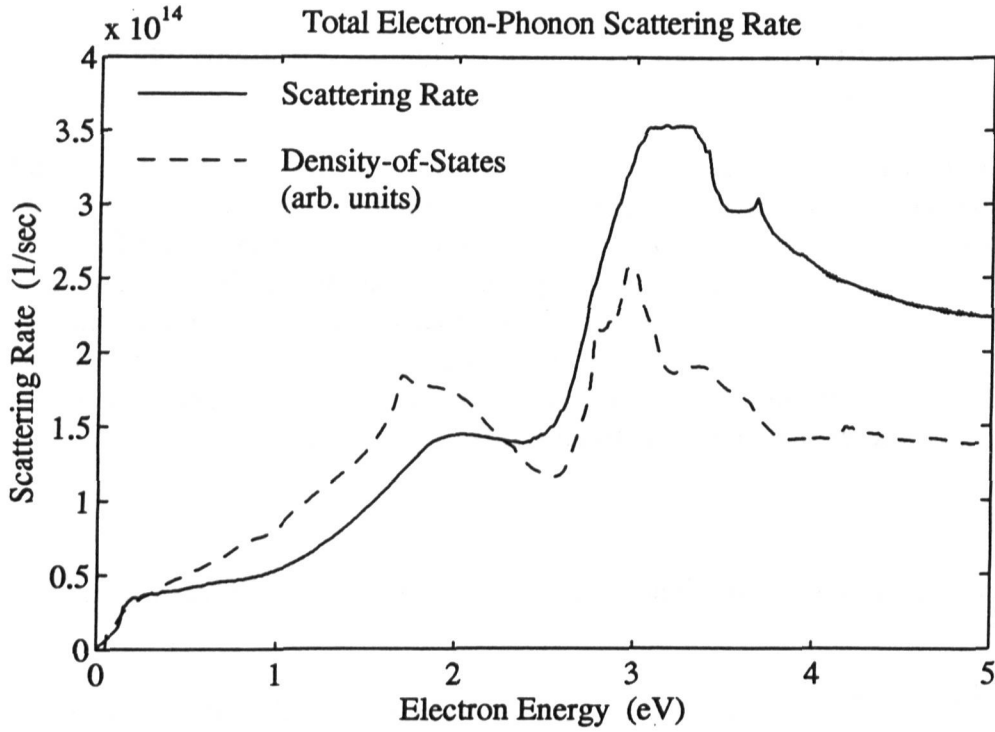


Fig. 1. Total electron-phonon scattering rate as a function of energy. Rates are into states in the first 4 conduction bands out of the first two.

adiabatic approximation, this is expressed as:

$$V_{el-ph}(\mathbf{r}) = \int d^3\mathbf{r}' \epsilon^{-1}(\mathbf{r}, \mathbf{r}'; \omega = 0) \sum_{j,\alpha} \delta\mathbf{R}_{j,\alpha} \cdot \nabla V_b^\alpha(\mathbf{r}' - \mathbf{R}_j - \tau_\alpha) \quad (5)$$

with transform [14]

$$V_{el-ph}(\mathbf{q} + \mathbf{G}) = \sum_{\mathbf{G}'} \epsilon^{-1}(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}'; \omega = 0) V_{el-ph,b}(\mathbf{q} + \mathbf{G}'), \quad (6)$$

defining

$$V_{el-ph,b}(\mathbf{r}) = \sum_{j,\alpha} \delta\mathbf{R}_{j,\alpha} \cdot \nabla V_b^\alpha(\mathbf{r} - \mathbf{R}_j - \tau_\alpha) \quad (7)$$

Under the assumption that the atomic pseudocharge density moves rigidly with the atoms of the crystal lattice under displacement, a linearized interaction potential reduces eq'n (5) to the inner product of the ionic displacement and the gradient of the screened ionic potential. In this case, the calculation of electron-phonon matrix elements proceeds closely along the lines of the standard rigid ion theory, with only minor modification.

III. Discussion

The method of [15] was used in conjunction with the Fermi Golden Rule and a realistic phonon dispersion to generate band- and wavevector-dependent electron-phonon scattering rates. Figure 1 shows the total energy-dependent scattering rate, with the density-

of-states included as a reference. The scattering rate is found to be larger than that of the empirical method [5], especially at high energies. As an indication of the anisotropy of these rates, figure 2 depicts an energy isosurface in the first conduction band, shaded proportionally to total rate at each point in the Brillouin zone.

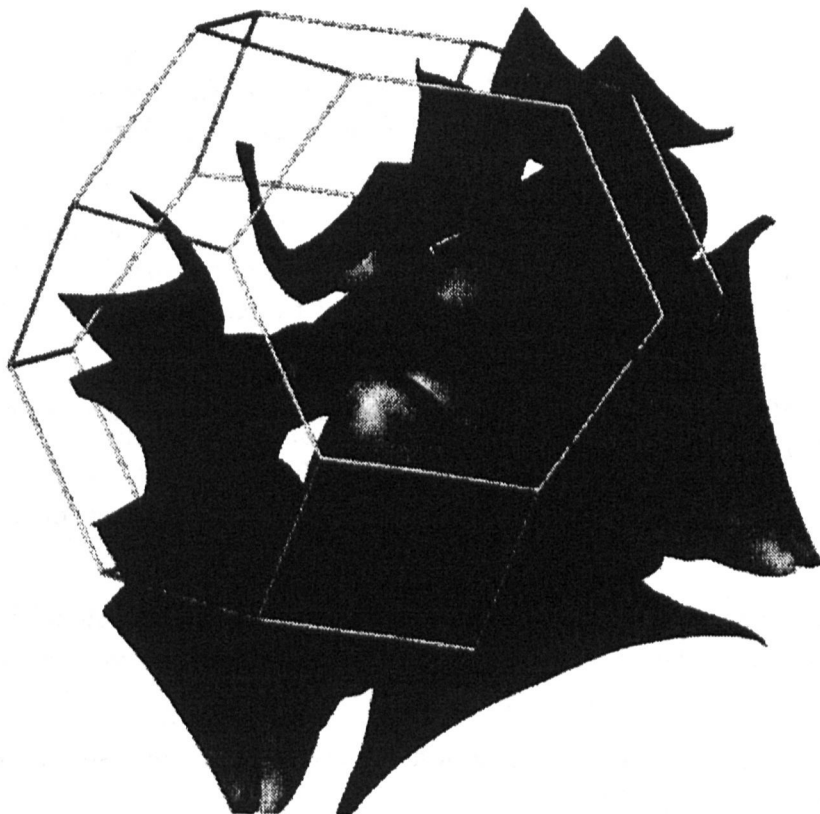


Fig. 2. Surfaces of constant energy ($=1.79$ eV), shaded by electron-phonon scattering rate in the lower half of the Brillouin zone. On these surfaces, the scattering rate varies by a factor of 3.94, indicating significant anisotropy.

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