Considerations on Treating Polar-Optical Phonon Scattering in Real Space

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ABSTRACT

For many applications, especially in quantum transport, a more accurate approach to handling scattering by the polar phonons may be had by a treatment in real space rather than by perturbation theory.

INTRODUCTION

In the treatment of carrier transport with quantum transport, non-equilibrium Green's functions are often used. These, however, have difficulty with scattering that arises from Coulombic centers, such as ionized impurities and the polar-optical phonons. In the case of impurities, much improved behavior is found by treating these centers in real space [1]. Importantly, it has been shown that this preserves the quantum coherence of the carriers during scattering [2]. Treating the polar-optical phonons by perturbation theory may well lead to difficulties with use of the non-equilibrium Green's functions, due to a need for the Bethe-Salpeter equation and disconnected diagrams in order to fully account for such phase coherence [3]. On the other hand, it has usually been assumed that optical phonon scattering led to complete phase breaking. Whether or not either view is completely correct only can be determined by treating the polar-optical interaction in real space.

MODEL

Here, semiconductors with the zinc-blende structure are considered. In this case, each atom of the A-B basis set is tetragonally coordinated with 4 nearest neighbors. An important point is that the polar LO mode corresponds to the two atoms in the basis oscillating against one another, as shown by the pair A_1-B in Fig. 1. While this one of the 4 neighbors is involved in the LO mode, it is important to understand that the other three atoms in the tetragonal bonding are moving with TO motion in conjunction with the B atom. Hence, the LO potential associated with the motion is a dipole potential (Fig. 2), where the dipole moment oscillates in time, and these potentials are oriented along one of the [111] axes of the crystal, and is coherent throughout the crystal due to TO modes.

The number of dipoles present (per unit volume) is given by the product of the Bose-Einstein distribution and the phonon density of states. In a simulation, the simulation volume is determined by the assumed density of carriers and the number of particles in the Monte Carlo simulation. Once the dipoles are introduced, in the same manner as discrete impurities, the particles are guided by the overall potential surface. One important point is that the dipole oscillates with a frequency of the LO mode, and this oscillation modulates the spatial shape of the potential and only weakly its amplitude. This oscillation determines the corresponding time step in the simulation.

Additionally, one has to address the exchange of energy between the carrier and the dipole. Excitation of excess phonons can increase the dipole amplitude, and this excess energy has to be allowed to either recombine or diffuse through the semiconductor.

CONCLUSION

A model for handling the polar-optical phonons in real space is proposed as one approach to such considerations.

REFERENCES

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[3] D. K. Ferry *et al*., *A Review of Quantum Transport in Field-Effect Transistors,* Semicond. Sci. Technol. **37**, 043001 (2022)

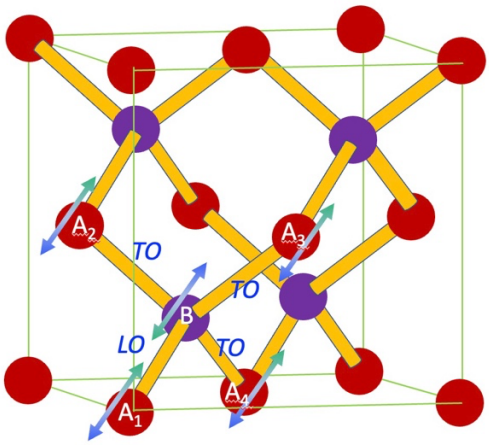

Fig. **1**. Motion of the atoms on one basis set may be the LO mode, simultaneously the other atoms in the tetragonal bonding are undergoing TO motion.

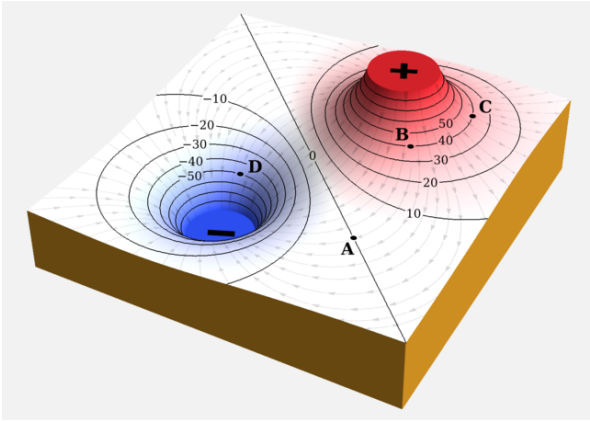

Fig. 2. A dipole potential. The dipole charge is aligned along the (111) crystal axis. (Wikipedia Commons 3.0)