

The many expression anharmonic lattice displacements in semiconductors

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I will discuss an unexplored, fundamental aspect in semiconductor (SC) physics - the effect of strongly anharmonic lattice dynamics on the electronic and optical properties of semiconducting materials.

Important macroscopic properties of SCs include charge carrier mobilities and lifetimes, optical absorption and emission (photo- and electro-luminescence). These macroscopic properties are usually described by approximated microscopic models that provide predictive power, intuitive understanding and important design rules for new materials. As it stands, the cornerstone of these models is the harmonic approximation which implies that the thermal nuclear motion in the solid can be described in terms of a finite number independent quantum harmonic oscillators.

The starting point of the analysis of lattice dynamics is a Taylor expansion of the crystal potential energy in terms of nuclear displacements from their equilibrium position. The first term vanishes and the second quadratic term is the harmonic contribution to the energy. Higher-order terms are classed together as anharmonic contributions. If the anharmonic terms are small in comparison to the quadratic term they are treated as a perturbation of the harmonic model. This approach is extremely useful as it allows deriving mathematical models that have exact solutions. In contrast, if the higher-order terms are not very small compared to the quadratic term, the potential surface becomes much more elaborate. Importantly, while the harmonic approximation has proven to work very well for traditional, tetrahedrally bonded, SCs such as silicon and gallium-arsenide, it fails to capture the structural dynamics of other types of SCs such as halide perovskites, organic crystals, and lead/tin-salts.

The halide perovskites are undoubtedly the most notable example for anharmonic SCs. Motivated by their recently discovered high PV efficiency, an intense research effort aimed to understand their fundamental properties is underway. Recent findings show that many of the halide perovskite's electronic properties such as very long carrier diffusion lengths/lifetimes, moderate carrier mobilities, very-low defect density, and even self-healing properties, do not follow traditional SC models and theories. I will show that the remarkable differences between halide perovskites and classic SCs stem from the strongly anharmonic lattice dynamics of the former.

Moreover, many more families of SCs are either shown or highly likely to exhibit anharmonicity. Organic SCs comprise a promising family of materials that have been intensively studied in the past decades for applications ranging from inexpensive PV cells to printable and transparent electronics. Inorganic ionic crystals such as lead and tin salts are efficient thermoelectric and mid-infrared detectors.

Despite the overwhelming evidence for strongly anharmonic lattice dynamics in many SCs, the effect of anharmonicity on their electronic properties is rarely considered. In my talk, I will discuss how anharmonicity is expressed in these materials with strong emphasis on electron-phonon interactions.