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A New Study of Polaron Scattering Phenomena in Bulk Semiconductor Devices

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Abstract— **It is shown that polaron scattering affects substantially the low-field electrical transport electron in bulk materials. It is found that the electron mobility decreases monotonically as the temperature increases. The important subcategories of polarons–large polarons, small polarons, and bipolarons–are considered in turn, along with the basic formulas and qualitative behaviors.**

Keywords-: *Polaron; bipolarons; electrical transport mobility.*

I. INTRODUCTION

The low-field electron mobility is one of the most important parameters that determine the performance of a field-effect transistor. The purpose of the present paper is to study the effect of polaron scattering on electrical characterizations [1-2]. The formulation itself applies only to the central Γ valley conduction band. We have also consider band non-parabolicity, admixture of p-type valence-band wave functions, degeneracy of the electron distribution to any arbitrary degree, and the screening effects of free carriers on the scattering probabilities. In a typical covalently-bonded crystal, electrons and holes can be characterized to an excellent approximation by assuming that they move through a crystal whose atoms are frozen into place. The electrons and holes can scatter off phonons, of course, but when no phonons are present at very low temperature all ionic displacement is ignored in describing electron and hole transport and properties.

This approach is inadequate in ionic or highly polar crystals where the Coulomb interaction between a conduction electron and the lattice ions results in a strong electron-phonon coupling.

II. LARGE POLARONS

In many materials, the radius of a polaron is much larger than the lattice constant of the material. In this case, the polaron is called a *large polaron*. The properties of such a polaron are parameterized primarily by a unitless number called the *Fröhlich coupling constant*, denoted α, defined by [3]

$$\alpha = \frac{e^2}{\hbar c}\sqrt{\frac{m_b c^2}{2\hbar\omega_{LO}}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \qquad (1)$$

where ε_0 is the static dielectric constant, ε_∞ is the high-frequency dielectric constant, m_b is the effective mass given by the band structure (i.e., not adjusted for polaronic effects), and ω_{LO} is the LO-phonon angular frequency. The parameter α is approximately twice the total number of phonons in the phonon cloud of a given electron or hole [2], and therefore polaronic effects are likely to start to become significant when α becomes order-unity or larger. In real crystals, measured values of α are in the range 0.02-0.2 for common III-V semiconductors, up to 0.3-0.5 in II-VI materials, typically 2-4 in alkali halides, and as high as 4.5 in the perovskite $SrTiO_3$ [4].

The effective mass of a polaron is larger than the mass of the underlying electron. Loosely speaking, the electron must drag the lattice distortion with it as it moves, creating a larger inertia. There is no known exact formula describing the mass increase, but one approximation due to Richard Feynman gives [5]:

$$m^* \approx m_b(1+\alpha/6) \qquad (2)$$

The mobility of a large polaron is often limited (at least in certain temperature ranges) by scattering due to (real) optical phonons, as a result of the strong electron-optical-phonon coupling in these materials. The number of (real) optical phonons in the material is proportional to $(\exp(\theta/T)-1)^{-1}$, where T is the temperature and $\theta=\hbar\omega_{LO}/k_B$ is the crystal's Debye temperature; therefore, the mobility is proportional to $(\exp(\theta/T)-1)$ [6]. More precisely, the mobility equals $F(\alpha)\exp(\theta/T)$, where F is a certain theoretically-predicted function [7]. This behavior is indeed seen in some polaronic materials, such as high-purity AgBr [8].

Large polarons have optical signatures in the THz frequency range (the frequency range where the photon frequency is comparable to ω_{LO}). For example, in a polaron, the electron