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Modeling of the annealing of radiation-induced defects in Germanium by moving discrete breathers

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Abstract

There is an increasing interest in the mechanism and properties of non-linear lattice vibrations in crystals, which may have large lifetimes and propagation distances, and are called intrinsic localized modes (ILM) or discrete breathers (DB) [1]. In recent theoretical works by some of the present authors, existence of sessile [2] as well as mobile DBs [3] have been demonstrated in metals by means of molecular dynamics using well defined MD potentials. An important peculiarity of this phenomenon is its low energy ranging from fractions to a few eV, which makes further investigations of low-energy collision events especially appropriate for various applications. Deep Level Transient Spectroscopy or DLTS is an especially useful technique for direct experimental observation of such phenomena in semiconductors, since it allows one to detect microstructural changes deep inside the material produced by low-energy collision events at the surface, which are analyzed in the present paper. We assume that moving DB can be trapped by structural defects thus creating trapped DB (TDB), which are shown to result in the amplification of the reaction rates involving the defects. The amplification mechanism has been proposed originally to explain anomalous low-temperature reconstructive transformations in layered silicates [4]. It is based on modification of the classical Kramers escape rate from a potential well due to a periodic modulation of the well depth (or the reaction barrier height). Then, a macroscopic reaction rate (averaged over a macroscopic number of defects) can be shown to depend on the frequency of the DB collisions with a defect resulting in the TDB formation (which is proportional to the irradiation flux) and the average TDB life-time, τ_{TDB}, during which the reaction is accelerated. Besides, it depends almost exponentially on the average TDB energy, E_{TDB}. A quantitative comparison of the model with experimental data on annealing of E-centers in Germanium by low-energy Ar plasma ($\sim$4 eV) [5] shows an excellent agreement at the following TDB parameters: $\tau_{\mathrm{TDB}} = 10^{-11}$ s , $E_{\mathrm{TDB}} = 0.62$ eV, which seem to be a reasonable estimate for the life-time and the mean energy of TDB produced by moving DB with energies ranging from 0.5 to 5 eV.

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