The Frozen Lattice Model:
Is it Valid to describe Thermal Diffuse Electron Scattering?

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Molecular dynamics simulations solving Newton's equations of many particle systems and using enhanced empirical potentials are performed to obtain frozen lattice (FL) models suitable for electron microscope image simulations [1, 2]. Snapshots of the atomic structures [3] are taken at equidistant times from a constant volume simulation (NVE ensemble), slightly rescaling all particle velocities to control the temperature up to the thermal equilibrium (cf. Fig. 1 for energy equilibration in a [100]-40x40x40GaAs-supercell with 216000 atoms). The simulated exit wave functions based on the FL's are transferred through the microscope with Gaussian distributed defoci describing the instabilities. Incoherent collection (cf. Fig.2, defocus half width 10nm around Scherzer, 200kV, Cs=1.2mm) of the intensities yields the phenomenon of thermal diffuse scattering (TDS). The semi-classical FL approach is justified because the atomic vibrations in a crystal (energies ≤ 0.1eV, velocities ≈ 10^3m/s) are much slower than the incident fast electron (100keV, 10^8m/s). If the incoherence is suitably considered and the specimen is thicker than the free mean phonon excitation path it is equivalent to a rigorous quantum approach [4]. However, by analyzing the vibrational spectrum a direct influence of the different phonon modes can be revealed in the images. A contrast mismatch between FL-simulated TDS and the usual approach using Debye-Waller factors corresponding to $\langle u^2 \rangle$ (cf. Fig. 1 and 2 insets), indicates whether phonon scattering is sufficiently considered [5,6]

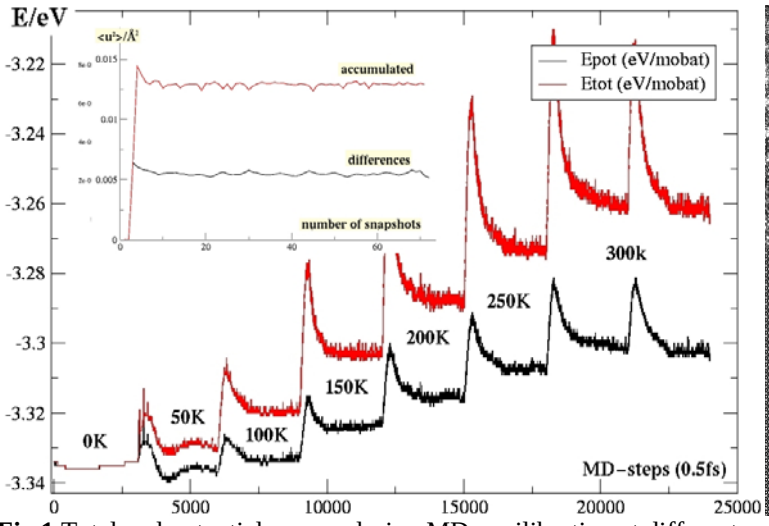

Fig.1 Total and potential energy during MD equilibration at different temperatures (in K). Inset: mean atomic square displacements of 300K.

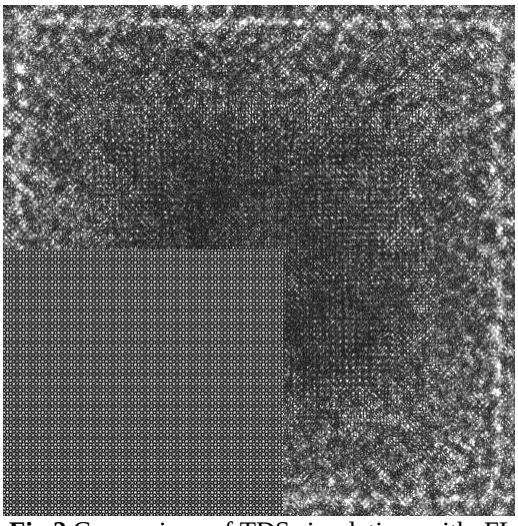

Fig.2 Comparison of TDS simulation with FL-approach and Debye-Waller description (inset).

References:

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[3] How to simulate TDS with MD relaxed frozen phonon states was discussed at the International Triebenberg Workshop in September 2003 near Dresden. All participants, but especially Harald Rose, are kindly acknowledged.

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