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Investigation of crystal defects by molecular dynamics simulations

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Several physical properties of crystalline materials, such as strength, electrical conductivity, magnetic, electronic, or optical properties, are fundamentally determined by the microstructure. The microstructure is characterized by the crystal defects, e.g. dislocations, as well as the grain and crystallite structure. Molecular dynamics (MD) methods are computer simulation algorithms that determine the motion of atoms and molecules by numerically solving equations of motion describing a multibody problem, starting from atomic potentials. These methods are very suitable for modelling the microstructure. These methods are applied to generate simulated diffraction patterns of crystals containing defects. The model based patterns are evaluated by the CMWP method, an experimental whole pattern modelling method which gives the relevant parameters of the microstructure. The input parameters of the MD method and the output parameters of the CMWP procedure are in good correlation. The efficiency of these methods is presented by solving various materials science problems.

Keywords: X-ray diffraction, line profile analysis, dislocations, molecular dynamics, modeling