Determination of Burgers Vectors from Atomistic Data

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ABSTRACT

Large-scale molecular dynamics simulations have been widely used to investigate the mechanical behavior of materials. But complex datasets, involving the positions of many million atoms, generated during the simulations make quantitative data analysis quite a challenge. This paper presents a novel method to determine not only dislocations in the crystal, but also to quantify their Burgers vectors. This is achieved by combining geometrical methods to determine the atoms lying in the dislocations cores, like for example the common neighbor analysis [1] or the bond angle analysis [2], with the slip vector analysis [3]. The first methods are used to filter out the atoms lying in undisturbed regions of the crystal; the latter method yields the relative slip of the remaining atoms and thus indicates the Burgers vector of those atoms lying in the dislocation cores. The validity of the method is first demonstrated on single edge dislocations in relatively small samples. Examples on large-scale atomistic simulations of nanoindentation reveal the full potential of the Burgers vector analysis. Furthermore a way will be sketched how this analysis can be used to determine densities of statistically stored and geometrically necessary dislocations, respectively. Hence, this method can be expected to provide valuable input for strain gradient plasticity models.

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