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BDA: A novel method for identifying defects in body-centered cubic crystals

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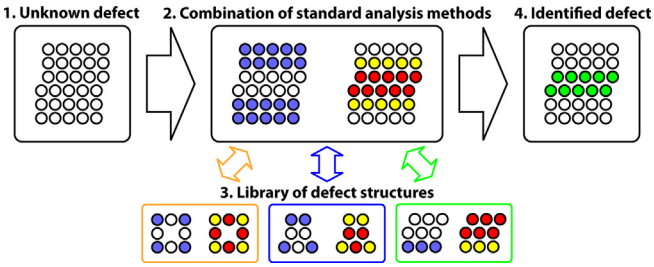
GRAPHICAL ABSTRACT



ABSTRACT

The accurate and fast identification of crystallographic defects plays a key role for the analysis of atomistic simulation output data. For face-centered cubic (fcc) metals, most existing structure analysis tools allow for the direct distinction of common defects, such as stacking faults or certain low-index surfaces. For body-centered cubic (bcc) metals, on the other hand, a robust way to identify such defects is currently not easily available.
We therefore introduce a new method for analyzing atomistic configurations of bcc metals, the BCC Defect Analysis (BDA). It uses existing structure analysis algorithms and combines their results to uniquely distinguish between typical defects in bcc metals.
In essence, the BDA method offers the following features:

- Identification of typical defect structures in bcc metals.
- Reduction of erroneously identified defects by iterative comparison to the defects in the atom's neighborhood.

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• Availability as ready-to-use Python script for the widespread visualization tool OVITO [http://ovito.org].

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Method

The interpretation and analysis of atomistic simulations of condensed matter hinges on the automatized identification of (lattice) defects [1,2], which is therefore a key element of many tools for atomic structure visualization [3–5]. While many different crystallographic parameters and algorithms have been developed for face-centered cubic (fcc) crystals [4,6], few methods are specifically adapted to the identification of defects in body centered cubic (bcc) crystals. An unambiguous, automatized classification of bcc crystal defects is of particular importance as large-scale atomistic simulations are increasingly used to study specific aspects of bcc plasticity and failure [7–10], including nanocrystal plasticity [11], dislocation-defect interactions [12–14], fracture [15], and in particular irradiation damage [16].

Here, we introduce a new method for analyzing atomistic configurations of bcc metals, the BCC Defect Analysis (BDA). It uses the results of the widely-used coordination number (CN), centrosymmetry parameter (CSP) [17], and common neighbor analysis (CNA) [18] to identify defects that are typical for bcc crystals. The first step within the BDA approach is to analyze all atoms in a given configuration with the CN, CSP, and CNA techniques. Here, it is noteworthy that the cutoff radius for the CN is $r_c = (1+\sqrt{2})/2a_0$ with a_0 being the lattice parameter. Since the six next-nearest neighbors of perfect bcc atoms are within this cutoff distance, their CN increases from 8 to 14. Then, the CN and CSP values of each atom, which is not in a bcc environment according to the CNA or has a CN of 14, are compared to empirically determined values for the following typical defects: surfaces, vacancies, twin boundaries, screw dislocations, {110} planar faults, and edge dislocations. The criteria for this pre-characterization are presented in the first three columns of Table 1.

The novelty of the BDA method is that not only the atom itself, but also each of its neighbors is evaluated against characteristic defect criteria. To this end, all atoms within the cutoff distance are classified according to their values of CN and CSP. N_p denotes the number of neighbor atoms being in a perfect bcc environment. The non-perfect neighbor atoms are compared to a number of different criteria, see the column nos. 5–9 in Table 1. If a neighbor atom fulfills a criterion, i.e., a certain combination of CN and CSP, the number N_d is increased for the respective criterion. If the occurrences of N_p and N_d match the characteristic occurrences for a defect, this defect is assigned to the atom. If not, the atom and its neighbors are evaluated against the criteria for the next defect in Table 1. This comparison is performed for all non-bcc atoms in the configuration. To minimize the number of erroneously identified defects, every identified defect is then compared to its neighboring defects and is flagged as 'unidentified' if it is not representing the relative majority among its neighbors. In the final step, all unidentified atoms are assigned to the predominant defect in their neighborhood. As a result, the number of unidentified defects is reduced by repeating this comparison until the number of unidentified defects is smaller than a threshold value or does not change upon further repetition. This step is optional, but recommended, since it homogenizes the resulting output data.

In essence, the BDA method consists of the following steps:

1 Calculate a-CNA [2], CSP [17], and CN (with cutoff radius $r_c = (1+\sqrt{2})/2a_0$ to include also next-nearest neighbors) for all atoms.
2 Generate list of non-bcc neighbors, i.e., with a-CNA$\neq$bcc or CN$\neq$14, for each atom.