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Data Article

Dataset illustrating the construction of dislocations and running dislocation dynamics using the periodic array of dislocation quadrupoles in FCC Al

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ABSTRACT

The data illustrates the process of creation of dislocation quadrupoles in FCC Al. The density of dislocations in our data is 3.8×10^{13} m^{-2} which is the lowest published to date and is comparable to the density of dislocations in real crystals. The data set can be found at the following URL:https://data.mendeley.com/datasets/mvmychgk4j/1. The detailed research article is "A topologically correct method of dislocations construction for atomistic modeling" (K. Yu. Khromov et al., 2019).

Specifications table

Subject area	Physics, Materials Science, Computational Materials Science
More specific subject area	Defect of the crystal structure, Dislocations
Type of data	*.tgz files
How data was acquired	The dump files were acquired by running LAMMPS [2] static potential energy minimization.
Data format	Raw, analyzed

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Experimental factors	The pretreatment consisted of creating an input file with the appropriate LAMMPS software commands.
Experimental features	The two steps procedure as described in detail in [1] was applied. First, an initial configuration was created by removing parts of atomic planes from a simulation volume. Next, LAMMPS was run to find a local minimum of potential energy corresponding to a dislocation quadrupole.
Data source location	Moscow, Russian Federation
Data accessibility	The data is in the Mendeley repository https://data.mendeley.com/datasets/mvmychgk4j/1
Related research article	K. Yu. Khromov, A. A. Kovalishin, V. A. Ryabov, T. V. Tsvetkov, V. E. Velikhov, "A topologically correct method of dislocations construction for atomistic modeling", Computational Materials Science, **156**, 301–309 (2019).

Value of the data

- The data is valuable for the construction of edge and mixed dislocations with realistic densities characteristic for real crystals even those not subjected to severe deformation.
- The data demonstrates an application of a new algorithm of the lowering of dislocation density by properly cutting a simulation volume and multiplying its parts farthest from dislocations.
- The data illustrates the advantage of using the quadrupole configurations for the construction of dislocations with an edge component when the periodic boundary conditions are used. The advantage manifests itself as much smaller deviations from the perfect crystalline structure, compared to the other methods of dislocations construction, at the boundaries of the periodic images.

1. Data

Al_disl.tgz is an archive with atomic positions. 1 × 512 × 128 and 1 × 1024 × 512 refer to the corresponding size of the simulations volume. The Al_edge_1 × 1024 × 512 directory contains gzipped files with the atomic coordinates acquired in the process of purely edge dislocation construction in FCC Al. The Al_mixed_1 × 512 × 128 contains files with the atomic coordinates acquired in the process of mixed dislocation construction in FCC Al. The files are visualizable using OVITO software [3].

2. Experimental design, materials and methods

The procedure for the preparation of the initial *.dat files containing atomic positions was described in the accompanying research article [1]. These files are in the format readable by LAMMPS software.

After the initial configuration is constructed, the atomic positions optimization is performed using LAMMPS *minimize* command. The files in the data archive are LAMMPS dump files saved at the intermediate stages of the optimization process. The columns in these files represent the following data (left to right):

- Atom number,
- Atom id,
- X position of the atom,
- Y position of the atom,

- Z position of the atom,
- The centro-symmetry parameter as described in LAMMPS documentation,
- The potential energy of the atom.

Acknowledgements

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.037.

References

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[2] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, J Comp. Phys. 117 (1995) 1–19 ⟨http://lammps.sandia.gov⟩.

[3] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO " the Open Visualization Tool", Model. Simul. Mater. Sci. Eng. 18 (2010) 015012 ⟨http://ovito.org⟩.