University of Groningen

Computed Structure of Grain Boundaries Compared with TEM Observations

Hosson, J.Th.M. De; Heringa, J.R.; Schapink, F.W.; Evans, J.H.; Veen, A. van

Published in:
Surface Science

DOI:
[10.1016/0039-6028\(84\)90699-X](https://doi.org/10.1016/0039-6028(84)90699-X)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
1984

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Hosson, J. T. M. D., Heringa, J. R., Schapink, F. W., Evans, J. H., & Veen, A. V. (1984). Computed Structure of Grain Boundaries Compared with TEM Observations. *Surface Science*, 144(1), 1-13.
[https://doi.org/10.1016/0039-6028\(84\)90699-X](https://doi.org/10.1016/0039-6028(84)90699-X)

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

COMPUTED STRUCTURE OF GRAIN BOUNDARIES COMPARED WITH TEM OBSERVATIONS

J.Th.M. DE HOSSON and J.R. HERINGA

Department of Applied Physics, Materials Science Centre, University of Groningen, Nijenborgh 18, 9747 AG Groningen, The Netherlands

F.W. SCHAPINK

Technological University Delft, Rotterdamseweg 137, 2628 AL Delft, The Netherlands

J.H. EVANS

Metallurgy Division, AERE Harwell, Oxon, UK

and

A. VAN VEEN

Interuniversity Reactor Institute, Technological University Delft, Rotterdamseweg 137, 2628 AL Delft, The Netherlands

Received 3 October 1983; accepted for publication 15 November 1984

Employing computer simulation techniques several studies of the relaxation of atoms in coincidence type grain boundaries have been performed in recent years. Often it is difficult to obtain a clear representation of the relaxed boundary structure, especially in the case of small atomic displacements. In this paper a method of representing the relaxed grain boundary structure is described using a Fourier analysis of the atomic configuration after relaxation. Computer experiments were carried out on $\Sigma = 19$, $46.8^\circ/[111]$ in Al. Next, results obtained from computer experiments dealing with the interaction between He and a tilt grain boundary in Mo are presented. Direct motivation for this study stems from the transmission electron microscopic observation of helium trapping at a set of $[100]$ edge dislocations defining a low angle tilt boundary in Mo.

EFFECT OF SECONDARY RELAXATIONS ON DIFFRACTION FROM HIGH- Σ $[001]$ TWIST BOUNDARIES

P.D. BRISTOWE and R.W. BALLUFFI

Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Received 3 October 1983; accepted for publication 15 November 1983

The types of diffraction effects which may be expected from secondary relaxations in high- Σ $[001]$ twist boundaries are calculated and discussed. An idealized two-plane model is used which incorporates secondary relaxations by rotating patches of boundary about coincident site lattice elements normal to the boundary. Local relaxations within the patches are also employed using rotational relaxations about local O-lattice elements in a manner consistent with earlier results. The main effect of secondary relaxations is the splitting of grain boundary reflections into small clusters which fall on a "grain boundary dislocation lattice". This localized splitting is significant only when the deviation of the boundary from a nearby low- Σ misorientation becomes sufficiently large. Under these circumstances a noticeable distortion of the diffraction pattern can also occur. The results are compared with some X-ray diffraction observations from twist boundaries in gold.