Springer Theses

Recognizing Outstanding Ph.D. Research

Aims and Scope

The series “Springer Theses” brings together a selection of the very best Ph.D. theses from around the world and across the physical sciences. Nominated and endorsed by two recognized specialists, each published volume has been selected for its scientific excellence and the high impact of its contents for the pertinent field of research. For greater accessibility to non-specialists, the published versions include an extended introduction, as well as a foreword by the student's supervisor explaining the special relevance of the work for the field. As a whole, the series will provide a valuable resource both for newcomers to the research fields described, and for other scientists seeking detailed background information on special questions. Finally, it provides an accredited documentation of the valuable contributions made by today's younger generation of scientists.

Theses are accepted into the series by invited nomination only and must fulfill all of the following criteria

- They must be written in good English.
- The topic should fall within the confines of Chemistry, Physics, Earth Sciences, Engineering and related interdisciplinary fields such as Materials, Nanoscience, Chemical Engineering, Complex Systems and Biophysics.
- The work reported in the thesis must represent a significant scientific advance.
- If the thesis includes previously published material, permission to reproduce this must be gained from the respective copyright holder.
- They must have been examined and passed during the 12 months prior to nomination.
- Each thesis should include a foreword by the supervisor outlining the significance of its content.
- The theses should have a clearly defined structure including an introduction accessible to scientists not expert in that particular field.

More information about this series at <http://www.springer.com/series/8790>

Thomas D. Swinburne

Stochastic Dynamics of Crystal Defects

Doctoral Thesis accepted by
Imperial College London, UK

Springer

Author

Dr. Thomas D. Swinburne
Theory and Modelling
Culham Centre for Fusion Energy
Culham Science Centre
Oxfordshire
UK

Supervisor

Prof. Adrian P. Sutton
Department of Physics
Imperial College London
London
UK

ISSN 2190-5053

Springer Theses

ISBN 978-3-319-20018-7

DOI 10.1007/978-3-319-20019-4

ISSN 2190-5061 (electronic)

ISBN 978-3-319-20019-4 (eBook)

Library of Congress Control Number: 2015942802

Springer Cham Heidelberg New York Dordrecht London

© Springer International Publishing Switzerland 2015

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made.

Printed on acid-free paper

Springer International Publishing AG Switzerland is part of Springer Science+Business Media
(www.springer.com)

Publications Related to This Thesis

Theory and simulation of the diffusion of kinks on dislocation lines in bcc metals, T. D. Swinburne, S. L. Dudarev, S. P. Fitzgerald, M. R. Gilbert and A. P. Sutton, Physical Review B, 2013 [1].

The work carried out by myself and reported in [1] is presented primarily in section 4.1 and Chap. 5.

Collective transport in the discrete Frenkel-Kontorova model, T. D. Swinburne, Physical Review E, 2013 [2].

The work carried out by myself and reported in [2] is presented primarily in section 5.5.

Thermally-activated Non-Schmid Glide of Screw Dislocations in W using Atomistically-informed Kinetic Monte Carlo Simulations, A. Stukowski, D. Cereceda, T. D. Swinburne and J. Marian, International Journal of Plasticity, 2015 [3].

The work carried out by myself and reported in [3] is presented primarily in section 4.1.4.

The classical mobility of highly mobile crystal defects, T. D. Swinburne, S. L. Dudarev and A. P. Sutton, Physical Review Letters, 2014 [4].

The work carried out by myself and reported in [4] is presented primarily in Chap. 6.

To Juliette

Supervisor's Foreword

The insight by Orowan, Taylor and Polanyi in 1934 that dislocations are the agents of crystal plasticity marked the beginning of the science of metallurgy. Since that time dislocations have played a central role in almost all mechanisms put forward to explain mechanical processes in crystalline matter. Dislocations are one of the 'big ideas' of materials physics.

Dislocations experience a variety of forces. Undergraduates learn about the Peach-Koehler force arising from the stresses acting on them. Much less attention is paid to the buffeting dislocations experience as a result of thermal fluctuations. These thermal forces are dominant when dislocation loops are at the nanoscale, and they are responsible for the Brownian motion these loops display in a transmission electron microscope. This is particularly significant in the context of radiation damage where point defects in steels cluster forming small nanoscale loops, which evolve into larger loops through this Brownian motion.

When they move dislocations experience friction from the crystal lattice. Earlier theories of the frictional force treated the dislocation as a defect in an elastic continuum interacting with phonons. More recently, molecular dynamics simulations have explored the dependence of the frictional force on temperature and the speed of the dislocation. The motivation for this work comes from a variety of sources. The velocity–stress relationship for dislocations is a crucial input into simulations of dislocation dynamics. However, current relationships are largely phenomenological interpretations of experiments or atomistic simulation with little theoretical understanding and thus predictive capability. The friction experienced by dislocations also plays a key role in models of fatigue crack nucleation, and in adiabatic shear where the intense heat generated by these frictional forces leads to an instability of strain localization, and in many other mechanical processes in crystals.

The frictional force and the thermal buffeting are two sides of the same coin. They are directly related by the fluctuation-dissipation theorem of statistical

mechanics. In this thesis Tom brings fresh insight into understanding the factors controlling defect mobility, especially dislocation mobility:

(a) By applying Zwanzigs projection techniques Tom explains analytically in the thesis the origin of the temperature-independent contribution to the lattice friction experienced by highly mobile defects such as crowdions, kinks on screw dislocations and small prismatic dislocation loops. His analysis resolved a long-standing disconnect between molecular dynamics (MD) simulations, which showed there was a contribution to the lattice friction experienced by nano-scale defects that was temperature independent, and 60 years of theory denying the existence of a temperature-independent contribution. Tom identified the terms responsible for the temperature-independent mobility and evaluated them, finding perfect agreement with his own MD simulations. As one referee of his Physical Review Letter [1] noted:

This paper fills an important gap in computational physics, namely, the determination of the origin of the temperature-independent friction coefficient from fundamental lattice dynamics, by convincingly separating the localized nature of defect cores from canonical vibrations. The theoretical arguments put forward by the authors are potentially applicable to many other areas in defect dynamics, and that should make this paper of interest to the general readership of PRL.

(b) In another original contribution Tom reproduced MD simulations of dislocation motion using a popular physics model, a harmonic chain sitting in a periodic potential agitated by random thermal forces [2]. This allowed dislocation simulations 107 times faster than MD, but no less accurate. This tremendous speed-up enabled him to simulate the kink motion of dislocations at realistic (experimental) levels of applied stress—an unprecedented achievement because these levels of stress are far too small to lead to any kink migration in standard MD simulations. His model revealed a previously unrecognised discrete length scale in dislocation dynamics, intermediate between that of the dislocation microstructure of conventional dislocation dynamics, and the atomic length scale of MD. In addition, Tom extended mathematical techniques of multi-scale analysis to gain new insight into the asymptotic time behaviour of this widely-studied model, providing connections between observed diffusion rates and the thermodynamic free energy barrier [3].

By any standards the originality and insight displayed in this thesis are exceptional. It is one of the finest examples of the work undertaken in the EPSRC Centre for Doctoral Training on Theory and Simulation of Materials at Imperial College, which was established in 2009 to attract physicists and engineers with a strong theoretical and/or computational prowess into materials science. There are further outstanding theses in the pipeline.

London
May 2015

Prof. Adrian P. Sutton

References

1. Swinburne TD, Dudarev SL, Sutton AP (2014) Phys. Rev. Lett. 113, 215501
2. Swinburne TD, Dudarev SL, Fitzgerald SP et al (2013) Phys. Rev. B 87, 064108
3. Swinburne TD (2013) Phys. Rev. E 88, 012135

Abstract

The state of a deformed crystal is highly heterogeneous, with plasticity localised into linear and point defects such as dislocations, vacancies and interstitial clusters. The motion of these defects dictate a crystal's mechanical behaviour, but defect dynamics are complicated and correlated by external applied stresses, internal elastic interactions and the fundamentally stochastic influence of thermal vibrations.

This thesis is concerned with establishing a rigorous, modern theory of the stochastic and dissipative forces on crystal defects, which remain poorly understood despite their importance in any temperature-dependent micro-structural process such as the ductile to brittle transition and irradiation damage.

From novel molecular dynamics simulations we parameterise an efficient, stochastic and discrete dislocation model that allows access to experimental time and length scales. Simulated trajectories of thermally activated dislocation motion are in excellent agreement with those measured experimentally.

Despite these successes in coarse graining, we find existing theories unable to explain stochastic defect dynamics. To resolve this, we define crystal defects through projection operators, without any recourse to elasticity. By rigorous dimensional reduction we derive explicit analytical forms for the stochastic forces acting on crystal defects, allowing new quantitative insight into the role of thermal fluctuations in crystal plasticity.

Acknowledgments

This is a welcome opportunity to sincerely thank Professor Adrian Sutton and Professor Sergei Dudarev for making my Ph.D. so enjoyable. I feel very lucky not only to have had access to two distinguished scientists with their constant intellectual agility and insight, but also to have had two receptive and responsive mentors who allowed me to take my own course whilst keeping me useful! I am very aware that under different guidance my mild idiosyncrasies could have seriously affected my scientific development, and their role in ensuring this did not happen cannot be overestimated.

The wider community at Imperial College (both Condensed Matter Theory and Theory and Simulation of Materials CDT) and CCFE have been fantastic environments; thanks in particular to Fabian Renn and Mark Gilbert for their endless patience with my numerous coding questions. I would also like to thank my thesis examiners, Dr. Peter Derlet and Dr. Gunnar Pruessner, for their critical reading of the submitted thesis and their resilience against the numerous spelling mistakes, which I hope have now all been corrected.

Finally, I give thanks to my parents for their constant support throughout my education and of course to my beloved Juliette for keeping my mind open, often through force.

TDS, April 2015, South Kensington, London

Contents

1	Introduction	1
	References	4
2	Dislocations	7
2.1	Topology and Burgers' Vector	8
2.2	Dislocation Core Structure	11
2.3	Dislocation Motion and the Kink Mechanism	12
2.4	Dislocations and Phonon Scattering Theory	13
	References	15
3	Stochastic Motion	17
3.1	The Langevin and Fokker-Planck Equations	17
3.1.1	Strong Damping Limit	19
3.1.2	State Dependent Damping	20
3.2	Projection Operators and the Mori-Zwanzig Technique	21
	References	25
4	Atomistic Simulations in bcc Metals	27
4.1	The Drift and Diffusion of Kinks	28
4.1.1	The Kink Vector	30
4.1.2	A Coarse Graining Procedure for Atomistic Simulation	30
4.1.3	Diffusion Simulations	33
4.1.4	Drift Simulations	40
4.2	The Drift and Diffusion of Lines and Loops	42
	References	46
5	Properties of Coarse Grained Dislocations	49
5.1	The Frenkel-Kontorowa Model	50
5.2	Langevin Simulation	52
5.3	Comparison of Parametrised Models to Experiment	55

5.4	Elastic Interactions in Double Kink Nucleation	57
5.5	Homogenisation of the Frenkel-Kontorowa Chain.	60
5.5.1	Adjoint Fokker-Planck Equation	62
5.5.2	Multiscale Analysis	63
5.5.3	Limiting Cases	69
5.5.4	Stochastic Simulation	71
5.5.5	Non-linear Response	72
	References	74
6	The Stochastic Force on Crystal Defects	77
6.1	The Projection Operator and Defect Coordinates	78
6.2	Derivation of Eshelby's Configurational Force	80
6.3	Removing the Vibrational Coordinates	81
6.4	Analytic Derivation	82
6.5	Numerical Evaluation	84
6.6	Discussion.	86
	References	87
7	Conclusions and Outlook	89
	References	90
	Appendix	91