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Vasily V Bulatov, Lawrence Livermore National Laboratory
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The Lawrence Fellowship, Lawrence Livermore National Laboratory (2001)
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Frederick E. Terman Fellowship, Stanford University (2004-2007)"

In the past twenty years new experimental approaches improved models and progress in simulation techniques have brought new insights into longstanding issues concerning dislocation based plasticity in crystalline materials during this period three dimensional dislocation dynamics dd simulations appeared and reached maturity their major objective is to contribute to the multiscale

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However this disparity can be attributed to the fact that murphy et al report the relative ordering of the dislocation energies at a distance 40 \AA from the dislocation line in atomistic simulations the dislocation energy as a function of radius is $e_{\text{tot}} \propto \frac{c}{r}$ at large distances from the dislocation line

Large scale first principles calculations were performed to determine the stability and mobility properties of screw dislocations in monosilicon carbide polytypes 4h 2h and 3c. Computer simulations of dislocations oxford series on materials modelling oxford university press new york 2006. Computer simulations of dislocations oxford series on materials modelling.

Weinberger S Aubry S W Lee and Wei Cai Dislocation Dynamics Simulations in a Cylinder Proceedings of the Dislocations 2008 International Conference IOP Conference Series Materials Science and Engineering Vol 3 012007 2009

This chapter introduces visualization programs and analysis tools that have been developed for working with the output of classical molecular dynamics and other atomistic simulation models. Basic analysis techniques relevant for nanomechanics problems are described which help to reveal structural phases, defects and local deformations. The plasticity of the fluorite structure in UO_2 is investigated with molecular dynamics simulation and empirical potential. The stacking fault energies and the dislocation core structures with burgers vector $a/2 [110]$ are systematically calculated. All dislocation core structures show a significant increase of the oxygen sub lattice disorder at temperatures higher than 1500 K.

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This book presents a broad collection of models and computational methods from atomistic to continuum applied to crystal dislocations. Its purpose is to help students and researchers in computational materials sciences to acquire practical knowledge of relevant simulation methods because their behavior spans multiple length and time scales. Crystal dislocations present a monoground for

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In conventional dislocation dynamics codes the motion of dislocations is entirely deterministic bulatov and cai puter simulations of dislocations 2003 the stochastic dislocation dynamics observed in md simulations and experimentally cannot be simulated with such codes

A parison of different continuum approaches in modeling mixed type dislocations in al modelling and simulation in materials science and engineering vol 27 issue 7 p 074004 puter simulation of liquids oxford university press new york 1989 55 verlet I puter experiments on classical fluids i thermodynamical. Molecular statics and molecular dynamics simulations are presented for the structure and glide motion of a 2 111 dislocations in a randomly distributed model bcc co 16 67 fe 36 67 ni 16 67 ti 30 alloy core structure variations along an individual dislocation line are found for a 2 111 screw and edge dislocations. Puter simulations of dislocations pdf part of the oxford series on materials modelling series download immediately available share description this book presents a broad collection of models and putational methods from atomistic to continuum applied to crystal dislocations. Dislocations mesoscale simulations and plastic flow ladislas kubin oxford series on materials modelling presents a prehensive coverage of the field with emphasis on the contribution of dislocation dynamics simulations.

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Abstract continuum dislocation theory cdt allows the consideration of dislocation ensembles by introducing the dislocation density tensor though the kinematics of geometrically linear cdt are well established the closure of governing field equations is not finished yet. Numerical simulations of crystal defects are necessarily restricted to finite putational domains supplying artificial boundary conditions that emulate the effect of embedding the defect in an effectively infinite crystalline environment this work develops a rigorous framework within which the accuracy of different types of boundary conditions can be precisely assessed. The conference series started on june 2000 at the national institute of standards and technology md usa since then dislocations conferences were held at la colle sur loup france in 2004 hong kong in 2008 budapest hungary in 2012 and at west lafayette in usa on 2016. Covid 19 resources reliable information about the coronavirus covid 19 is available from the world health organization current situation international travel numerous and frequently updated resource results are available from this worldcat search oclc s webjunction has pulled together information and resources to assist library staff as they consider how to handle coronavirus.

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