Physical modeling on size-dependent yield strength with dislocation pile-up and surface effects in finite single-crystal samples

Bo Pan, Yoji Shibutani

Department of Mechanical Engineering, Osaka University, Suita, 565-0871, Japan

Experimental and theoretical researches have shown their explanations of size-dependent relationship between steeply increasing yield strength and decreasing sample size [1-2]. But few researches focus on describing the dislocation pile-up effect and the surface effect in single-crystals on the size effect.

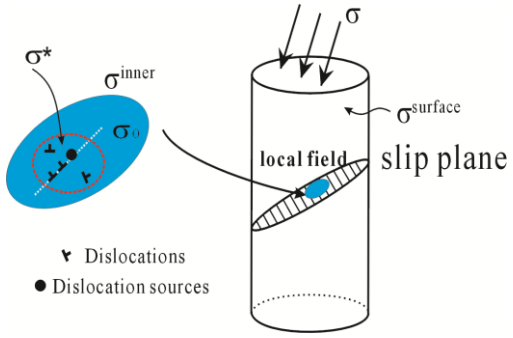

Figure 1: A schematic sketch of stresses state by considering both the surface effect and the micro effect of inner microstructures. The external stress needs to bypass the surface stresses and then be regarded as the applied stresses applied on the inner field to activate inner microstructures.

In this work, a physical model of the yield strength of finite single-crystals at the micrometer scale is derived from the inner microstructure effect and the surface effect as shown in Fig.1. The yield stress σ can be written as $\sigma = \sigma_0 + \sigma^* + \sigma^{surface} = \sigma^{inner} + \sigma^{surface}$, where σ^* and σ_0 are the stresses affected and not affected by dislocations, respectively [3]. Based on the principle of minimum potential energy, the surface stress $\sigma^{surface}$ can be derived as: $\sigma^{surface} = \gamma O_0 (1-\nu)/A$, where γ is the surface energy density, O_0, A are the perimeter and area of the initial cross section and ν is the Poisson's ratio. According to the dislocation pile-up configuration, the inner strength σ^{inner} can be obtained by considering the effect of microstructures, such as effective length of dislocation source $\bar{\lambda}_{\max}$, dislocation pile-up length L, dislocation density ρ_0, the number of dislocation sources and so on. It can be expressed as: $\sigma^{inner} = (\alpha\mu b/\sqrt{L\bar{\lambda}_{\max}} + \tau_0 + 0.5\mu b\sqrt{\rho_0})/SF$, where τ_0 is Peierls-Nabarro force, α is the geometric parameter, *SF* is the Schmidt factor, also μ and *b* are the shear modulus, and the Burgers vector, respectively. In this case, the stress of the filed can be finally obtained as

$$\sigma = \sigma^{inner} + \sigma^{surface} = (\alpha\mu b/\sqrt{L\bar{\lambda}_{\max}} + \tau_0 + 0.5\mu b\sqrt{\rho_0})/SF + \gamma O_0(1-\nu)/A \qquad (1)$$

It is shown that the "Hall-Petch" relation holds even in the single-crystal, and the number of dislocation pins is a significant factor in the size effect [4]. The process of simulations indicated that the starvation of dislocation sources is one reason for the observed size effect. Moreover, an explicit relationship between the stacking fault energy and the effect of dislocation pile-up was determined in this study: materials with low stacking fault energy will exhibit an obvious dislocation pile-up effect. Furthermore, it can be found that the surface effect from the geometries and the inner strength from the inner microstructures interplay each other, and both influence on the yielding strength, which has the size-dependent characteristic.

[1] D.M. Dimiduk, M.D. Uchic, T.A. Parthasarathy, Acta Mater. **53**, 4065 (2005).
[2] T.A. Parthasarathy, S.I. Rao, D.M. Dimiduk, et. al, Scripta Mater. **56**, 313 (2007).
[3] J. Wang, Y. Cui, X. Feng, et. al, Europhys Lett. **92**, 16002 (2010).
[4] B. Pan, X. Zhang, K. Yukihiro, F. Shang, Y. Shibutani, submitted to JAP.

Modeling thermal activation of dislocation glide in cementite at low temperature

Nils Garvik, Philippe Carrez, Patrick Cordier

Unité Matériaux et Transformations, UMR CNRS 8207, Université de Lille 1, 59655 Villeneuve d'Ascq Cedex, France

For a better understanding of mechanical properties in pearlite, we propose to study plastic deformation in cementite. Under extreme deformation, iron carbide Fe_3C (orthorhombic structure, described in the following using *Pnma* space group) exhibits lamellar structure refinement of pearlitic steels [1]. At low temperature and high stress, experimental results show that cementite can deform with [100] dislocations spreading on (010) with dissociation in two partial dislocations separated by a stacking fault [2].

Due to experimental limitations, we propose a numerical model of dislocation core structures and mobility, through an evaluation of associated critical resolved shear stress (CRSS). Our calculations rely on a Peierls-Nabarro-Galerkin model to describe complex core structures at the atomic scale using, as an input, first-principles calculations for generalized stacking fault (GSF) energies [3]. It should be pointed out that how carbon atoms are allowed to relax during GSF energies calculations has a strong effect on stacking fault energies (i) but also on dislocation core structure (ii).

i) Restoring force, derived from stacking fault energy, are in good agreement with previous ideal shear stress calculations [4,5].
ii) Dislocation core structures are in agreement with experimental observations, with a dislocation of Burgers vector [100] spread in (010). Moreover, the dissociation width and partial Burgers vectors are found in good agreement with experimental data [2].

We identify two potential slip systems [100](010) and [001](100). In the low temperature, high-stress regime, cementite deformation is driven by the thermally activated motion of dislocations over the Peierls barriers through the nucleation and propagation of kink-pairs. We use the line tension model to describe kink-pair geometry [6,7] and the temperature dependence of the critical resolved shear stress (CRSS) of those two slip systems.

[1] K. Hono et al., Scr. Mater. **44** (2001)
[2] L. E. Kar'kina et al., The Phys. Metals Metall., **114** (2013)
[3] C. Denoual, Phys. Rev. B **77** (2008)
[4] N. Garvik et al., Mater. Sc. Eng. A **572** (2013)
[5] C. Jiang,S. G. Srinivasan, Nature **496** (2013)
[6] A. Seeger, Dislocation (1984)
[7] T. Suzuki et al., "Dislocation dynamics plasticity" **12** (1991)

M111 dislocation of high Peierls stress in BCC Ta

Sanghyuk Yoo[1], Keonwook Kang[1], Christopher Weinberger[2], Wei Cai[3], Vasily V. Bulatov[4]

[1]Dept. of Mech. Engr., Yonsei University, Seoul, 120-749, S. Korea
[2]Dept. of Mech. Engr., Stanford University, Stanford, CA94305, USA
[3]Mech. Engr. & Mechanics, Drexel University, Philadelphia, PA 19104, USA
[4]Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Dislocation mobility is a key factor to influence plastic behavior of materials, and can be measured by Peierls stress calculation. Peierls stress (PS) is the critical stress at which an infinitely long dislocation starts to move at 0K, and is regarded as intrinsic lattice resistance to dislocation motion. Using atomistic simulations, we calculated PS of a <111>/2{110} dislocation in a model system of BCC Ta with more than 100 different line orientations [1], among which two high PS orientations are identified: one at screw and the other at M111. While the highest PS at screw has been reported several times in many journal articles, the importance of 2nd highest PS at M111 orientation seems to be taken less seriously. In order to show that this observation is universal regardless of interatomic potential models, we have used two typical potential types of FS [2-4] and EAM [5] and the results are compared with ab initio calculations. All simulations results are consistent in that PS at M111 orientation is on the order of several hundreds MPa. This considerably high PS at M111 creates unique faceting motion in dislocation and is believed to be responsible for pre-yielding in BCC materials.

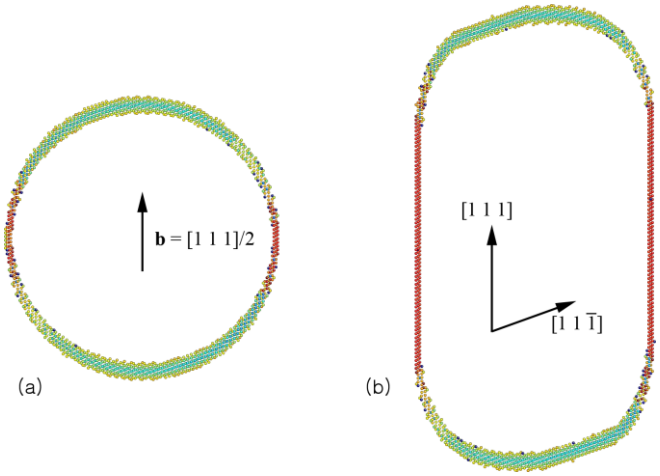

Figure 1: Molecular dynamics images of a dislocation loop of **b**=[111]/2{110} in BCC Ta. (a) Initial circular loop (b) The loop expanded under shear stress of 1 GPa at T = 10K. The loop develops in a faceted motion, clearly showing two distinct orientations: screw and M111

This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education (2013R1A1A2063917). The computations in this work were partly performed at the Supercpmputing Center/Korea Institute of Science and Technology Information with supercomputing resources including technical support (KSC-2013-C1-026).

[1] K. Kang, V.V. Bulatov, and W. Cai, PNAS, **109**, 15174 (2012).
[2] M.W. Finnis and J.E. Sinclair, Philos. Mag., **50**, 45 (1984)
[3] M.W. Finnis and J.E. Sinclair, Philos. Mag. A, **53**, 161 (1986)
[4] G.J. Ackland and R. Thetford, Philos. Mag. A, **56**, 15 (1987)
[5] X.W. Zhou, R.A. Johnson, and H.N.G. Wadley, Phys. Rev. B, **69**, 144113 (2004)

Studying the Effect of Stress Relaxation and Creep on Lattice Strain Evolution of Magnesium Alloy AZ31 under Tension and Compression

H. Wang, B. Clausen, C.N. Tomé, I.J. Beyerlein

Los Alamos National Laboratory, Los Alamos, NM, US

Three approaches for in-situ neutron diffraction measurements, namely, strain holding, stress holding and continuous event-mode, are used to measure the lattice strain evolution of magnesium alloy AZ31 rolled plate under both tension and compression. Stress relaxation or creep induced by holdings is inevitable, especially at loads which are close to the flow stress of the material and affects the results of the measurements. The effect of stress relaxation or creep on the evolution of the lattice strain is studied via comparison with the continuous measured results. To this effect, the experiments are simulated and interpreted using the elastic-visco-plastic self-consistent (EVPSC) polycrystal model in conjunction with an evolving dislocation density (DD) hardening law and a twinning and de-twinning (TDT) twin scheme. The predictions are in reasonable agreement with the corresponding measurements and provide insight into the stress relaxation mechanisms in Mg alloys.

To be presented at International Conference on Multiscale Materials Modeling to be held in San Francisco on October 6 to 10, 2014

Ab initio investigation of the Peierls potential of screw dislocations in bcc iron and its consequences on the dislocation-carbon interaction

L. Ventelon[1], L. Dezerald[1], F. Willaime[1], E. Clouet[1], L. Proville[1], D. Rodney[2]

[1]CEA, DEN, Service de Recherches de Métallurgie Physique, 91191 Gif-sur-Yvette, France
[2]Institut Lumière Matière, Université Lyon 1, CNRS, UMR 5306, 69622 Villeurbanne, France

The high yield stress and the subsequent low ductility in body-centered cubic (bcc) transition metals (V, Nb, Ta, Mo, W, Fe) originate from the core properties of screw dislocations with ½<111> Burgers vector, which lead to high energy barriers between two minima. Ab initio electronic structure calculations now allow us to quantitatively describe this barrier, so-called the Peierls barrier. More generally the topology of the 2D Peierls potential of <111> screw dislocations in all bcc transition metals is being revisited by density functional theory (DFT) calculations. Our DFT results yield 2D Peierls potentials very different from the usually assumed landscapes. We show that iron has a specific and surprising behavior compared to the other bcc transition metals, with a monkey saddle instead of a local maximum located at the hard core, while the energy of the split core configuration is on a high energy peak of the Peierls potential as for the other bcc transition metals [1, 2].

This new picture of the Peierls potential in iron, and in particular the low energy of the hard core, has major consequences on the dislocation-solute interaction in iron. The interaction between a screw dislocation and an interstitial carbon atom is investigated for various solute positions in the vicinity of the dislocation core. It is found that this interaction is strong enough to locally induce an inversion of the stability of the hard versus easy core configurations. A low energy configuration is indeed found where the solute atom is trapped at the center of the dislocation core in the hard core configuration, forming a carbon centered regular trigonal prism similar to the cementite building unit. These new findings have an important impact on the carbon enrichment on dislocations and on the effect of carbon on dislocation mobility.

[1] L. Ventelon, F. Willaime, E. Clouet and D. Rodney, Acta Mater. 61 (2013) 3973.
[2] L. Dezerald, L. Ventelon, E. Clouet, C. Denoual, D. Rodney and F. Willaime, Phys. Rev. B 89 (2014) 024104.

Predicting the Rate of Dislocation Cross Slip in FCC Metals

William P. Kuykendall[1], Keonwook Kang[2], Jie Yin[3], Wei Cai[1,3]

[1] Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA
[2] Department of Mechanical Engineering, Yonsei University, Seoul120-749, South Korea
[3] Department of Materials Science and Engineering, Stanford University, Stanford, USA

Cross slip is of fundamental importance for dislocation multiplication, strain hardening, fatigue, and dynamic recovery processes. Because cross slip in FCC crystals is a rare event on the atomistic time scale, it is a challenge to accurately predict the rate of cross slip from atomistic models. A major difficulty arises from the fact that multiple stress components influence the cross slip energy barrier. For the first time, we computed the energy barrier for homogenous cross slip of screw dislocations in FCC metals (Ni[1] and Al) as a function of three stress components, including the Schmid and Escaig stresses on the cross slip plane, and the Escaig stress on the original glide plane. These calculations required the development of a modified string method for stability at high stress conditions. The energy barrier data computed for hundreds of stress combinations are found to be well described by a one-dimensional function of an "effective stress", which is a linear combination of the three stress components. The regions in the stress space in which different cross slip mechanisms (e.g. Friedel-Escaig and Fleischer) operate are delineated. The effect of jog on the stress dependence of cross slip energy barrier is also discussed.

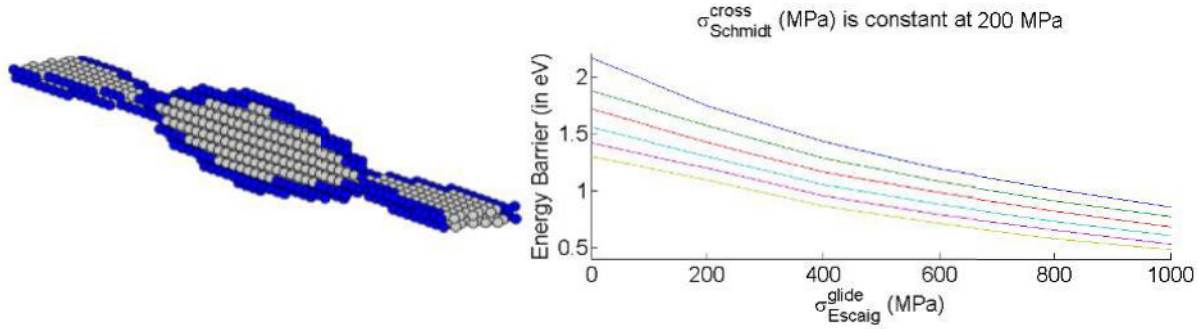

Figure 1: Left: Atomistic simulation of cross slip by the Friedel-Escaig mechanism. Right: The energy barrier (in eV) for homogenous cross slip as a function of increasing Escaig stress on the glide plane (x-axis) and increasing Escaig stress on the cross slip plane (different curves, lower curve is higher stress, in increments of 200MPa, starting at 0 MPa). The Schmid stress on the cross slip plane is fixed at 200 MPa. Other stress components are zero.

This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0010412.

[1] K. Kang, et al., J. Mech. Phys. Solids, **62**, 181-193, (2014).

Molecular dynamics simulation of dislocation motion in high-entropy alloys

S. Q. Wang

Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS, Shenyang 110016, P. R. China

As the development of superalloys is close to their application limit, the high-entropy alloy is emerging as the most promising candidates for next-generation high-temperature materials [1]. Toughness and ductility are the two key factors for structual application of a material. All of the two properties are close related with the dislocation movement in the solid. The dislocation structure and property in FCC CoCrFeMnNi and BCC AlCoCrFeNi high-entropy alloys are studied by computer simulations in this work. Different to the usual crystalline solids, high-entropy alloy is paracrystalline phase in which there are neither long-range translational nor rotational symmetries but only a certain fixed neighboring relationship among its lattice sites. Lattice distortions are everywhere in paracrystals [2]. Figure 1 shows the typical paracrystalline lattice of AlCrCuFeTiZn high-entropy alloys.

The atomic configurations of conventional edge and screw dislocations in FCC CoCrFeMnNi and BCC AlCoCrFeNi are built by the first-principles ground-state geometric optimization within the density-functional theory based on the bulk models of these phases [3]. The distribution of strain field around a single dislocation of each types is analyzed.

Figure 1: Paracrystalline lattice in AlCrCuFeTiZn high-entropy alloys.

Molecular simulations are performed using the Morse pair potentials created by Chen's lattice inversion method for the quantitative predictions of dislocation mobility in these two high-entropy alloys. A edge dislocation dipole is created by removing a layer of atoms in the rectangular box of FCC CoCrFeMnNi and BCC AlCoCrFeNi. The periodic boundary condition is used, and a Parrinello-Rahman shear stress is applied to make the dislocation motion [4]. The effects of lattice distortion to the dislocation movement in FCC CoCrFeMnNi and BCC AlCoCrFeNi high-entropy alloys are comparatively studied.

This work was supported by the National Basic Research Program of China (No. 2011CB606403) and the National Natural Science Foundation of China (No. 50971119).

[1] D. B. Miracle, *et. al.*, Entropy. **16**, 494 (2014).
[2] S. Q. Wang, AIP Advances. **3**, 102105 (2013).
[3] S. Q. Wang, Entropy. **15**, 5536 (2013).
[4] J. Chang, *et. al.*, Comput. Mater. Sci. **23**, 111 (2002).

Grain Scale Models of Plasticity in BCC iron: Describing the Role of Temperature, Strain Rate and States of Stress on Yield

Christopher R. Weinberger[1], Hojun Lim[2], Corbett C. Battaile[2], Lucas M. Hale[3], Jonathan A. Zimmerman[3]

[1]Drexel University, Philadelphia, PA
[2]Sandia National Laboratories, Albuquerque, NM
[3]Sandia National Laboratories, Livermore, CA

Plasticity in BCC metals, including iron, is known to exhibit strong temperature and moderate rate sensitivity in their flow stresses, and the orientation dependent flow stresses in single crystals deviate from the well known Schmid Law. In a related presentation (by Jonathan Zimmerman), atomistic simulations are described that predict the kink-pair activation enthalpy as a function of stress in BCC iron.

Through an appropriate normalization technique, a universal law that describes the orientation dependent yield stresses is developed, and these results can be integrated into higher length-scale models.

We will describe the integration of these results into a crystal plasticity model for BCC iron that captures the experimentally observed rate and temperature dependence as well as the atomistically parameterized stress dependence. The model is able to correctly reproduce the stress dependent yield observed in experiments that cannot be explained by a simple Schmid Law. This model is also used to investigate how to integrate hardening from dislocation-dislocation interactions with the stress-dependent lattice resistance. Using strain hardening behavior fit to experiments from the literature, the model is then used to investigate the role of temperature on the shape of the yield surfaces for both single- and poly- crystals. Our results show that the polycrystalline behavior of BCC iron yield surfaces quickly converges to the standard Von Mises yield surface as temperature is raised above 0K, with no noticeable differences above ~100K.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Probing Micro-Mechanics of Flow in Metals through Crackling Noise and Mean Field Theory

Xiaoyue Ni[1], Gabriele Vajente[2], Eric Quintero[2], Fei Sun[3], Rana Adhikari[2], Karin A. Dahmen[3], Julia R. Greer[1]

[1]Division of Engineering and Applied Sciences, California Institute of Technology, Pasadena, California 91125-8100, USA
[2]Department of Physics, California Institute of Technology, Pasadena, California 91125-8100, USA
[3]Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080, USA

One important aspect of mechanical behavior of materials is establishing a link between micro-mechanics of crystalline deformation and macroscopic plasticity. This is in part because testing theoretical predictions at the appropriate length scale is challenging because of the limited strain sensitivity in nano-mechanical instruments. We developed a methodology to study the internal dynamics of materials driven by defect activity when the sample is subjected to macroscopic deformation. This setup is based on a Michelson interferometer, with the target displacement resolution of order 10^{-15} m/$\sqrt{\text{Hz}}$ in the range between 10 and 10^3 Hz. We focus on "crackling noise", which arises from a nonlinear conversion of energy from slow varying external condition to high-frequency random events that are correlated with defect activity: dislocations or shear transformation zones. We aim to reliably obtain the crackling noise data from a variety of materials and interpret it in the context of micro-mechanics and defect activities at the micro-structural level. Statistical Mean-Field Theory (MFT) is used to both analyze the data and to develop predictions about across-the-scales behavior in terms of proximity to critical stresses.