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APPLICATIONS OF MICRODYNAMICS AND LATTICE MECHANICS TO PROBLEMS IN PLASTIC FLOW AND FRACTURE

Final Report - (4/1/73 - 3/31/78)

Prepared on 6/21/78

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DISCLAIMER

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INTRODUCTION

This final report summarizes the accomplishment made during the past five years while under Contract EY-76-S-02-3476 from Energy Research Development Administration (now Department of Energy) for the investigation of the application of microdynamics and lattice mechanics to the problems in plastic flow and fracture. The research program consisted of both theoretical formulations and experimental measurements of a number of intrinsic material parameters in bcc metals and alloys including surface energy, phonon-dispersion curves for dislocated solids, dislocation-point defect interaction energy, slip initiation and micro-plastic flow behavior.

The research performed was part of an international program undertaken corporatively at the State University of New York at Stony Brook, Stony Brook, New York, and the Politecnico di Milano, Istituto di Ingegneria Nucleare, CESNEF, Italy. As indicated by the amount of joint publications, student and post-doctoral exchange between both laboratories, and the international summer schools organized by scientists from both parties, the international cooperation has been a fruitful one.

THEORETICAL INVESTIGATION

As an approach to correlate atomistic and mechanical properties of materials, theoretical work has been performed toward an interpretation in terms of lattice dynamics of some relevant parameters, such as the surface energy for brittle fracture, the Peierls stress of a dislocation, the drag stress affecting the dislocation mobility, and the core energy of a dislocation. An essential theoretical tool developed in the course of this program was to exploit the knowledge of the interplanar and the interatomic force constants, available through neutron inelastic scattering.

The basically irreversible process of cleavage may be described in terms of a phase transition approach. Under the applied mechanical stress, the perfect lattice configuration of the crystal becomes unstable. This occurs when the spearation of the atomic planes in a particular direction reaches locally a critical value preliminary to interplanar separation; other configurations of the system then become possible, eventually resulting in a pair of free surfaces. In this frame, the surface energy, γ, for brittle fracture was initially explored in terms of the energy needed to load the interplanar force constants up to a critical value corresponding to melting followed by boiling. More recently this critical value has been the object of a more accurate assessment extended also to non-monoatomic systems using, instead of the melting-boiling concept, a criterion for mechanical instability of a system of rigid planes coupled by a realistic interplanar potential function.

This approach has been adopted to study the surface energy of cubic metals (5), alkali halides (8), and the ceramic MgO material (11). Qualitatively the results indicate the correct cleavage systems for all cases and quantitatively are reasonably consistent with the available experimental values.

Interplanar force constants play an important role also in the interpretation of the glide systems in crystals and in the determination of the Peierls stress σ_p, which is defined as the maximum value of the applied stress necessary to move the unit length of the dislocation line from the stable to the unstable configuration (2,4,5,7). Of course, many dissipative mechanisms are active when the dislocation is moving. However, low values of σ_p in certain directions of slip indicate an intrinsic dynamic sensitivity of the crystal to easily glide in those directions. The relevant parameter governing σ_p appears to be the ratio K/A, where K is the interplanar transverse (or shear) force constant, effective between planes parallel to the slip plane, and A is the longitudinal interplanar force constant related to the planes perpendicular to the slip plane. The lower the K/A ratio, the lower also σ_p. The model has been applied to fcc and bcc metals, and the results have been compared with those obtained in the frame of the isotropic continuum model leading to an improved insight into the dynamics of dislocation motion.

The model, with some modifications, can also be applied to study dislocation mobility and the interaction of a uniformly moving single edge dislocation with the non-rigid substrate of the containing crystal. In this way one can study the phonon contribution to the drag stress

and the corresponding stress-velocity relationship for a moving dislocation as a function of temperature. The results may also be satisfactorily compared with the data on the viscous damping constant obtained in ultrasonic attenuation measurements (9).

Dislocations, like point defects, alter the vibrational properties of a lattice also by creating resonance and localized modes (16,34,41). No experimental evidence exists up to now for such modes due to the difficulty of preparing suitable samples,and to the lack of an adequate theory predicting where in reciprocal space and time the dislocation-induced modes should be searched. This problem has been considered in connection with conceivable inelastic neutron scattering experiments aiming at the determination of the phonon dispersion curves of the localized modes associated with a screw dislocation in a model simple cubic lattice. The numerical evaluation of the local mode cross-section has been carried out for several scattering directions over a range of values of the involved interatomic force constants and as a function of dislocation density. Although the results indicate that the cross-section still lies at the borderline of detectability, the measurement of these dislocation modes is shown to be important, as it provides a means for evaluating the core energy of screw dislocations, without reference to precise knowledge of the lattice potential.

EXPERIMENTAL INVESTIGATION

(a) Surface Energy of bcc Metals & Alloys

Experimental measurements of fracture surface energy in single crystals of tungsten, molybdenum, niobium, and molybdenum-niobium alloys have been made using crack propagation techniques (15, 17, 18, 33).

In these experiments an initially sharp crack is introduced into the specimens by electric spark erosion techniques* . The propagation of this crack at liquid nitrogen temperatures upon loading allows an estimate of γ for the crystallographic plane of crack propagation. Some effort has also been initiated in accounting for the effect of plastic deformation at the crack-tip (44,45).

(b) Effect of Interstitial Concentration on Dislocation Dynamics in Molybdenum & Tungsten

Localized obstacles to dislocation motion in tungsten and molybdenum single crystals from 4.2°K to 298°K have been studied using compressional microstrain techniques (24,31,40). Ultrahigh vacuum electron bombardment purification techniques have been used to reduce both the dislocation and interstitial content. Techniques based on the measurement of residual electrical resistivity ratio and partial pressure gas mass spectrometry allow an estimate of impurity contents. Etch-pitting techniques were used to directly correlate microstrain observations with dislocation generation and motion (6). It has been found that edge dislocation generation and movement are active in the microstrain region while screw dislocations are relatively inactive until the macrostrain is reached. In molybdenum, dislocation velocity range from 10^{-6} to 10^{-3} cm/sec and the average distance between interstitial impurity pinning points is found to be ~8×10^{-4} cm in purified sample.

(c) Dislocation Dynamics in Copper & Copper-Nickel Alloys

Ultrasonic attenuation measurements were made using a pulse-echo technique in Cu-Ni alloys for a wide range of solute concentrations and dislocation densities (25,33,38). The solute concentrations were varied

*Beardmore, P. & Hull, D., J.Inst.Metals, 94, 14 (1966)

over 4 orders of magnitude from 0.01 to 10.0 at .% Ni, to study the influence of solutes on the dislocation damping parameters. The micro-structural effects were studied by changing the dislocation density over two orders of magnitude from $\approx 10^6/cm^2$ to $\approx 10^8/cm^2$, in a controlled manner. The dislocation densities were measured using etch-pit methods to correlate the damping parameters with the micro-structure.

The results indicate that the dislocations in Cu-Ni alloys are fully saturated with solutes at very low concentrations of Ni (<0.1 at .%). The dislocation damping constant, B, is found to be a sensitive function of the inherent dislocation content of the material. A change in dislocation density by ≈ 2 orders of magnitude produces a change in the B coefficient by about the same amount. The damping constant of pure undeformed copper at room temperature was found to be 3.9×10^{-5} dynes-sec/cm^2. A change in the Ni solute concentration by 4 orders of magnitude does not change the B coefficient of Cu very significantly. The room temperature B values of undeformed Cu-Ni alloys are lower than those reported earlier. This could be accounted for by a possible difference in dislocation densities of the crystals used in the two separate studies.

It is concluded that the B coefficient has a strong structural contribution and a relatively weaker solute contribution. In order to understand the solute effects on the dynamical behavior of dislocation motion in a random localized obstacle field, one must necessarily separate the strong micro-structural effects which may tend to obscure the real solute effects. When this is done, the presence of Ni solutes is found to affect the damping capacity or the frictional forces on moving dislocations in Cu, but the magnitude of this solute effect is

small. The concentration dependence of the structure normalized damping constant (B/Λ) is weak and is proportional to 0.073 power of the Ni concentration. These results argue in favor of a dislocation-phonon interaction as the governing mechanism for the source of frictional forces against dislocations in random localized obstacle fields.

CONCLUSIONS

The research supported by this grant has resulted in an improved understanding in the relationship among the experimentally determined fracture surface energy, the intrinsic cohesive energy between atomic planes, and the plastic deformation associated with the initial stages of crack propagation. The values of intrinsic surface energy of tungsten, molybdenum, niobium and niobium-molybdenum alloys, deduced from the measurements, serve as a starting point from which fracture toughness of these materials in engineering service may be intelligently discussed.

The motion of dislocations in purified crystals of low dislocation density demonstrates the ease of plastic flow in these materials when localized obstacles to slip have been removed from the host lattice. It is expected that crack nucleation and propagation will be greatly impeded when such conditions are fulfilled. The techniques developed for alloy crystal growth and ultrahigh vacuum annealing should be of interest in other future research in bcc metals and alloys.

The resistance to dislocation motion in fcc copper and copper-nickel alloys of well-characterized micro-structure demonstrated the inadequacy of existing theories in accounting for the observed mechanical damping. It has been shown that the effect of dislocation content may

be as important as the effects of solid solution hardening in some instances.

Local phonon modes in defect crystals has been shown to exist in model crystals. The identification of the frequencies of these modes should serve as a guide for their detection in future experiments. The significance of these caluclations lies in the possibility of future studies on the nature of the dislocation core structure.

Personnel Supported on Grant

Name	Position Held	Date
Bilello, J.C.	Associate Professor	1973-1974
	Professor	1974-1976
	Acting Associate Dean, College of Engineering & Applied Sciences	1976-1977
	Dean, College of Engineering & Applied Sciences	1977-present
Liu, J.M.	Post Doctoral Research Associate	1973-1976
	Visiting Assistant Professor	1976-1977
	Assistant Professor	1977-present
Boffi, S.	Visiting Consultant from Politecnico di Milano, Istituto di Ingegneria Nucleare, CESNEF	Annually
Caglioti, G.	Visiting Consultant from Politecnico di Milano, Istituto di Ingegneria Nucleare, CESNEF	Spring semester 1976
Bottani, C.E.	Visiting Consultant from Politecnico di Milano, Istituto di Ingegneria Nucleare, CESNEF	Sprin
Dralla, J.R.	Research Assistant	1973
Banerji, S.	Research Assistant	1973-1974
Pucino, A.	Research Assistant	1973-1978
Desko, J.	Research Assistant	1973-1977
Berkowitz, B.	Research Assistant	1973-1974
Kwok, D.N.	Research Assistant	1974-1976
Glass, H.	Research Assistant	1974-1976

Name	Position Held	Date
Weinstein, D.	Research Assistant	1975-present
Shen, B.W.	Research Assistant	1976-present
Mitchell, T.	Research Assistant, Visiting from Imperial College, London	1977-(summer)

Exchange Personnel from SUNY Stony Brook to Italy:

Banerji, S.	Post-doctoral Fellow at the Politecnico di Milano	1974
Glass, N.E.	Research Fellow at the Politecnicodi Milano, and U. of Pavia	1976

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