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A novel constitutive model for semiconductors: The case of silicon

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ABSTRACT

The photovoltaic industry relies heavily on solar-grade silicon multicrystals. Understanding their mechanical behavior requires the development of adequate constitutive models accounting for the effects of both high dislocation densities and complex loading situations in a wide range of temperature, strain rate, and impurity contents. The traditional model of Alexander and Haasen poses several limitations. We introduce in this work a novel constitutive model for covalent single crystals and its implementation into a rate-dependent crystal plasticity framework. It is entirely physically based on the dislocation generation, storage and annihilation processes taking place during plastic flow. The total dislocation density is segmented according to the dislocation mobility potential and their character. A dislocation multiplication law for the yield region more accurate than the one of Alexander and Haasen is proposed. The influence of additional dislocation sources created on forest trees, usually disregarded in models for semiconductors, is assessed. The dislocation velocity law combines three potentially rate-limiting mechanisms: the standard double kink mechanism, jog dragging and the influence of localized obstacles. The model is valid at finite strains, in multiple slip conditions and captures accurately the high temperature- and strain rate sensitivity of semiconductors. The experimental stress overshoot is qualitatively reproduced only when jog dragging is accounted for. Localized obstacles are shown not to have any significant effect on dislocation motion in silicon. The broader case of extrinsic semiconductors is discussed and the influence of dissolved oxygen on the upper yield stress of silicon monocrystals is successfully reproduced.

1. Introduction

1.1. Current approach

1.1.1. The yield region of semiconductors

Dislocations in semiconductors, in particular silicon, have received a special interest as these materials can be produced virtually defect-free and dislocations studied individually. The dynamical properties of dislocations in silicon have been

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Nomenclature

AH	Alexander and Haasen
$a_{\alpha\beta}$	coefficients depending on the interaction parameters
$A_{\alpha\beta}, B_{\alpha\beta}$	constant interaction parameters
a	lattice parameter
$\mathbf{b}$	Burger's vector
c_j	jog density
C	material constant in the AH model
C_O	dissolved oxygen concentration
d_j	mean jog spacing
D_{sd}	self-diffusion coefficient
D_O	effective diffusion coefficient of oxygen in the silicon matrix
$\mathbf{E}^e$	Green–Lagrange strain tensor
f_α	group of forest systems relative to system α
$\mathbf{F}$	deformation gradient
$\mathbf{F}^e$	elastic deformation gradient
$\mathbf{F}^p$	plastic deformation gradient
ΔG_O	binding energy of oxygen to the dislocation
h_{max}	maximum dipole height
h_{min}	minimum dipole height
ΔH_O	enthalpy change
l_f, l_v, l_{FR}	mean free path
l_{obs}	mean distance between obstacles
$\mathbf{L}^p$	plastic velocity gradient
k_b	Boltzmann's constant
K_1	multiplication law constant referring to increase in dislocation density due to expansion of existing dislocation loops on the slip plane
K_2	constant relating to the generation of new loops from forest interactions
K_{FR}	a coefficient related to f_α
m	material constant in the AH model
$\mathbf{n}_0$	normal unit vector
n_j	number of jogs per unit volume
r_a	capture radius
$\mathbf{R}^p$	rotation of the material element induced by plastic flow
t_w	waiting time
ΔS_O	entropy change
$\mathbf{s}_0$	unit vector in the slip direction
$\mathbf{S}^e$	the second Piola–Kirchoff stress tensor
T	temperature
U	material constant in the AH model
U_{LD}	effective activation energy for dislocation motion in the length-dependent regime
$\mathbf{U}^p$	plastic stretch tensor
v	dislocation velocity
v_0	velocity prefactor
v_{CH}	applied crosshead speed
$\overline{v}$	mean dislocation velocity
v_{dk}	dislocation velocity by the double kink mechanism
v_{jog}	velocity of jogged dislocations
X	dislocation length
X_c	thermally activated critical dislocation length
α, β	slip system
θ	angle of the velocity vector
μ	shear modulus
ν	Poisson's ratio
λ_O	constant related to oxygen diffusion to the dislocations
$\mathcal{L}$	fourth-order stress tensor
κ_+	a parameter characterizing the effective jog density actually affecting dislocation motion
$\dot{\gamma}$	shear strain rate
$\dot{\gamma}_p$	plastic shear strain rate
τ	applied shear stress
τ_0	a normalizing stress
τ_0^{ref}	a reference stress for normalizing purpose
τ_O	back stress caused by the dissolved oxygen
τ_O^{min}	minimum locking stress required for impurities to have a significant effect on the mobile dislocation density
τ_{uy}	resolved upper yield stress
τ_{ly}	resolved lower yield stress
τ_{int}	internal stress
τ_{eff}	effective stress
$\overline{\tau}_{eff}$	mean effective stress
ρ_i	immobile dislocation density
ρ_m	mobile dislocation density
ρ_t	total dislocation density
ρ_{ref}	reference forest density
ρ_{obs}	obstacle density
Ω	atomic volume

studied extensively since Patel and Chaudhuri (1963) revealed the characteristic yield drop of the flow stress upon dynamical straining of as-grown crystals. This behavior is *a priori* not limited to semiconductors but to any material presenting a deficit of mobile dislocations upon loading as discussed by Estrin and Kubin (1986). Too few dislocations limited in their motion by the high Peierls potential of the diamond cubic lattice cannot accommodate the imposed strain rate, resulting in an apparent elastic behavior of the crystals until an explosive dislocation multiplication allows for relief of the flow stress and the occurrence of a yield drop (for reviews see, e.g., Alexander and Haasen, 1968; George and Rabier, 1987; George, 1987).

The properties of the yield region, also called stage 0 of deformation, have been studied extensively throughout the years (Patel and Chaudhuri, 1963; Yonenaga and Sumino, 1978; Omri et al., 1987 to mention but a few). Its extent and the intensity of the yield drop are enhanced at low temperatures, high strain rates and low initial dislocation densities. The resolved upper yield stress τ_{uy} is found very sensitive to sample prestraining and its surface state, whereas the lower yield stress τ_{ly} is almost solely determined by the temperature and strain rate, provided the initial dislocation density remains low enough to avoid disturbing effects from the forest as mentioned by Yonenaga and Sumino (1978), Suezawa et al. (1979) and Siethoff