DYNAMIC BEHAVIOR OF MANY-DISLOCATION SYSTEMS IN SILICON

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Summary Dynamic behavior of dislocations in silicon crystals deformed at constant strain rates is simulated using a two-dimensional discrete-dislocation model. The model consists of infinitely repeated cells, each of which contains the same number of positive and negative mobile dislocations. Calculated results indicate that the experimentally observed *steady state of deformation* corresponds to the dislocated state that maximizes the mean internal stress on moving dislocations.

INTRODUCTION

Semiconductor is a rare kind of material where both the mobility of individual dislocations under stress and the state of collective dislocation motion during its macroscopic deformation have been obtained experimentally by highly reliable methods. Mechanical behavior of a silicon crystal deformed at a constant strain rate has several noticeable features [1]. Among them, the appearance of a *Steady State of Deformation* (SSD) is particularly remarkable. The SSD appears shortly after the lower yield point and continues at least throughout stage I of the stress-strain curve. In this state the value of effective stress, which corresponds to the mean of the stresses acting on all the moving dislocations in the crystal, remains constant irrespective of increase in strain and in dislocation density. The steady value of the effective stress depends on deformation condition (strain rate and temperature), but not on the initial density of dislocations nor on deformation history of the crystal before the SSD begins.
Although it has been a long time since the SSDs were discovered first in germanium crystals and later in silicon and other semiconductor crystals [1][2], the fundamental problems of why and how the states appear and are determined by deformation condition have not been solved completely yet. There have been studies [3]-[5] on the problems in terms of mean field quantities of stresses and dislocation densities, but no attempt was made on the basis of interactions between many discrete dislocations.
As a step toward physical understanding and solution of the problems, the present study simulates dynamic behavior of discrete dislocations in silicon crystals under constant strain rates, using a two-dimensional model of many-dislocation systems.

MODEL

The model crystal consists of infinitely repeated rectangular cells, each of which has a length L in X-direction and a height H in Y-direction and contains N ($N/2$ positive and $N/2$ negative) mobile straight dislocations having the same Burgers vector, with N being an even number (Fig.1). The dislocations are parallel to Z-axis and glide on slip planes parallel to X-Z plane. Configuration of N dislocations within each cell is the same. Under an *applied stress* τ_{a} or a uniform external shear stress acting on the slip planes and in the slip direction (parallel to the Burgers vector), the dislocations move in positive or negative X-direction. In order to focus on how the interaction between mobile dislocations affects dynamic behavior of many-dislocation systems, multiplication and annihilation of dislocations are not considered.
In the present study, a constant total shear strain rate $\dot{\gamma}$ with respect to the slip system is imposed at and after time $t=0$ as a deformation condition; temperature is kept constant at 800 degrees centigrade. A density of dislocations ρ in the crystal is given as a material condition. If these conditions, the cell size, and an initial configuration of dislocations in a cell are given, we can obtain dynamic behavior of the N dislocation system by solving a system of differential equations in $N+1$ unknown functions of t, *i.e.*, in τ_{a} and N x-values of dislocations in a cell.
The cell size was chosen to be $L = 40\,[\mu\mathrm{m}]$ and $H = N/(L\rho)$. Four kinds of cell (P, Q, R, and S) were prepared, whose H values were given by this relation from four experimental values [2] of moving dislocation density in the SSDs at imposed strain rates $\dot{\gamma}_{\mathrm{P}} = 2.4\times10^{-5}[\mathrm{s}^{-1}]$, $\dot{\gamma}_{\mathrm{Q}} = 1.2\times10^{-4}[\mathrm{s}^{-1}]$, $\dot{\gamma}_{\mathrm{R}} = 2.4\times10^{-4}[\mathrm{s}^{-1}]$, and $\dot{\gamma}_{\mathrm{S}} = 6.0\times10^{-4}$ $[\mathrm{s}^{-1}]$. Configuration of N dislocations in a cell ($N=30$) in a cell at $t=0$ was obtained by using uniform pseudorandom numbers. M initial configurations ($M=7$) were considered for each of four kinds of cell. Dislocations were assumed to have screw character, because motion of screw dislocations is rate controlling in plasticity of silicon crystals [1].

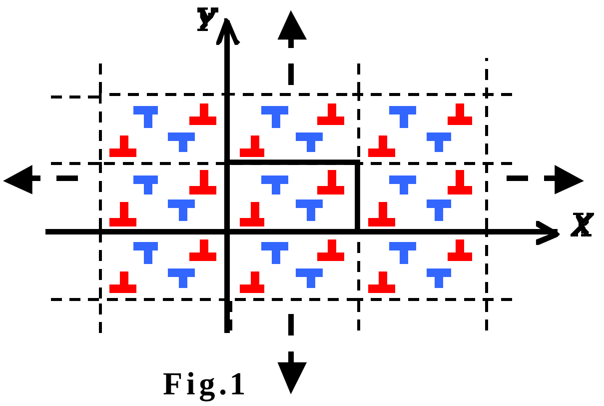

Fig.1

RESULTS AND DISCUSSION

A *dislocation average* of effective stress, $<\tau_{eff}>$, is defined by the mean of effective stresses acting on N dislocations in a cell of a dislocation system at time t. Fig.2 shows an example of the changes in τ_a and $<\tau_{eff}>$ with time in cell Q starting from a certain initial configuration of dislocations and deformed at strain rate $\dot{\gamma}_Q$. Several seconds after the start of deformation, $<\tau_{eff}>$ comes to fluctuate around a constant value of stress. Two horizontal lines in the figure indicate time averages of τ_a and $<\tau_{eff}>$ over the time interval 40 to 100[s], which are called *T-averages* and denoted by τ_{aT} and $<\tau_{eff}>_T$ respectively. *Configuration averages* (C-averages) $<\tau_{aT}>$ and $<<\tau_{eff}>_T>$ are defined as the mean of τ_{aT} and $<\tau_{eff}>_T$ respectively over M many-dislocation systems with different initial configurations.

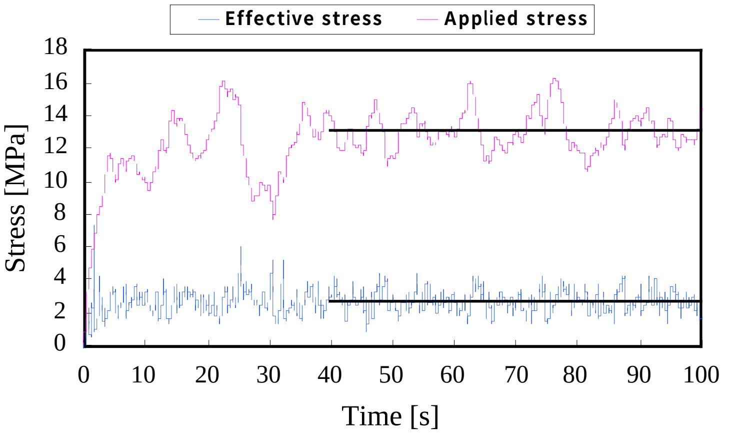

Fig.2

Fig.3 shows strain rate dependence of $<<\tau_{eff}>_T>$ in cells P, Q, R, and S. The calculated mean effective stress at each of four circled points in the figure equals the experimental value of effective stress in the SSD at each strain rate. Strain rate dependence of the experimental effective stress in the SSD is significantly different from that of calculated one in any of the cells. The discrepancy should come from the fact that moving dislocation density ρ_{mov} changes autonomously in deformation of Si crystals, while in the simulation such change does not occur and instead the density of mobile dislocations in each cell is fixed.

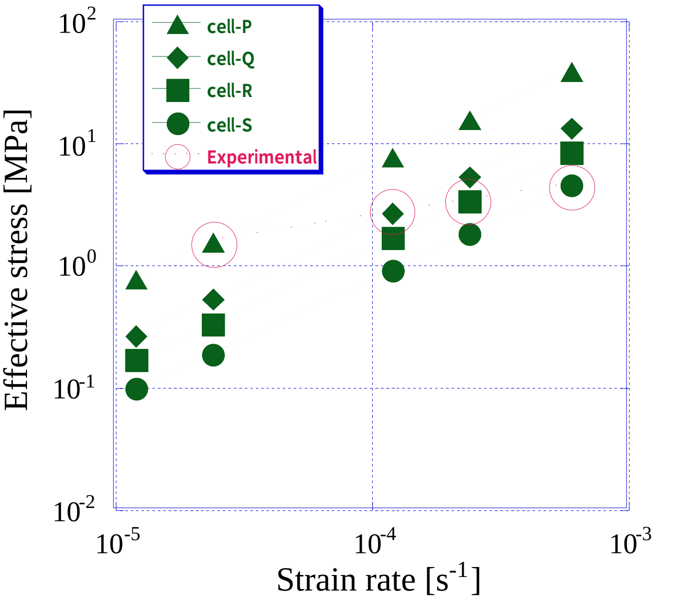

Fig.3

In Fig.4, C-averages of internal stress (applied stress minus effective stress) acting on moving dislocations in cells P, Q, R, and S are plotted against strain rate. As in Fig.3, the strain rate at each of the four points circled corresponds to the deformation condition when each cell was prepared.

What is most striking here is that each circled point lies at the maximum of the strain rate dependence curve for each cell. This indicates that the SSDs found in experiment correspond to the dislocated states that maximize the mean internal stresses on moving dislocations.

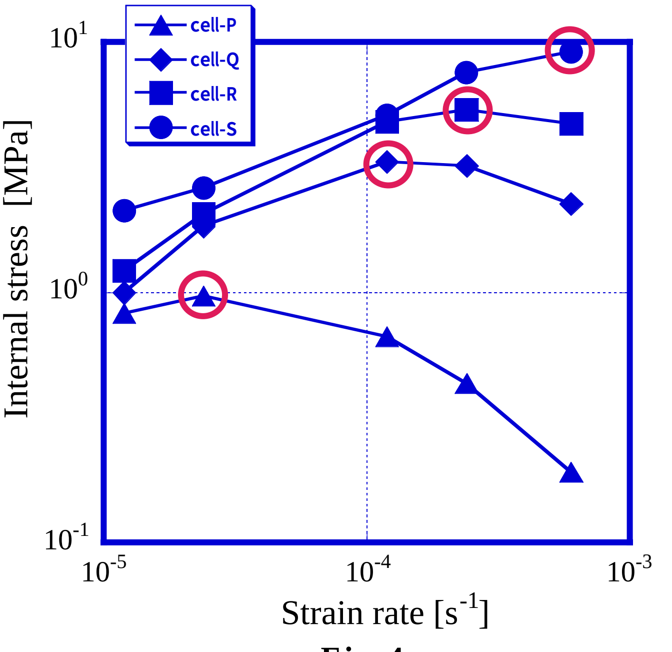

Fig.4

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