Constitutive modeling of intrinsic silicon monocrystals in easy glide

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Constitutive modeling of silicon materials is currently restricted to the very early stage of deformation. Uniaxial tensile testing of monocrystals oriented for single glide is traditionally simulated by a scalar model relying on the so-called machine equation. The present work uses a crystal plasticity framework to identify the role of secondary slip systems in the yield region. A three-dimensional finite element model of a tensile apparatus is validated by comparison of its outputs to the results yielded by a scalar formulation. Best fits of the constitutive model of Alexander and Haasen to experimental data reveal strong variations in its parameters with temperature. An improved constitutive model for intrinsic silicon monocrystals deformed in single glide is described. Its parameters are identified as analytical functions of temperature. We show its excellent agreement with the observed steady state of deformation in stage I.

I. INTRODUCTION

Silicon is an attractive semiconductor for production of cost-efficient photovoltaic (PV) solar cells because of its availability and suitable band gap, allowing efficient power generation. Silicon-based modules account nowadays for the largest share of the commercial PV market and are expected to remain the leading technology for the years to come.

Silicon is submitted to several thermomechanical loadings during its purification and processing, such as ingot solidification and cooling, wafer cutting, and the successive heat treatments aimed at increasing cell efficiency. Mechanical loadings at high temperatures are conveniently relaxed by plastic deformation, but eventually generate residual stresses in the material that can ease fracture later on the production line, silicon being brittle at room temperature. The prediction of the response of silicon to a thermomechanical loading path would help assessing the amount of plastic deformation in the crystals and improve our understanding of fracture events.

The constitutive models available in the literature are traditionally derived from the work of Alexander and Haasen (AH model in the following). It successfully describes the yielding behavior of as-grown silicon monocrystals of low initial dislocation density deformed uniaxially in single glide. The initial apparently elastic deformation is followed by an intense drop of the flow stress due to the fast multiplication of dislocations in the crystal, called yield drop. Estrin and Kubin showed that such an effect is not typical to silicon monocrystals but rather to materials presenting a deficit of mobile dislocations upon loading, relative to their saturation density. Silicon crystals are nonetheless peculiar due to the covalent bonds between their constituent atoms leading to high Peierls valleys and a strong lattice friction opposing dislocation mobility. It follows a significant dependency of the mechanical response of silicon materials to strain rate and temperature, as observed experimentally.

As-grown crystals have extremely low primary dislocation densities (typically 10⁸ m⁻²). The AH model assumes consequently that all dislocations are mobile and that short-range interactions are inexistent. Forest dislocations being considered absent, the classical models of hardening describing the storage of dislocations as a function of a mean free path (for example, see Refs. 8 and 9) are not applicable.

An adequate description of the yield drop requires an appropriate law for the evolution of the dislocation density with deformation. Models for fcc crystals rely on dislocation multiplication, stemming from the activation of Frank–Read sources in the crystals. Recent investigations on germanium crystals have proposed a generic multiplication law. We will consider in this paper the generation law typically mentioned as workable in the case of silicon. Dislocation dynamics simulations have provided with a new law for dislocation multiplication, stemming from the activation of Frank–Read sources in the crystals. Recent investigations on germanium crystals have proposed a generic multiplication law.
use a crystal plasticity framework to allow the potential activation of secondary systems through the yield region and evaluate its intensity. The constitutive equations of Alexander and Haasen as well as the extensions we suggest in this paper are introduced in Sec. II. The crystal plasticity framework in which any of those material models can be implemented is briefly exposed. Section III concentrates on the ways uniaxial tensile tests can be simulated with the help of a three-dimensional (3D) finite element model or a scalar model, respectively. The identification of the constitutive parameters of the AH model in Sec. IV points out to their significant and partly unphysical temperature dependence. The improvements brought by our constitutive model are shown in Sec. V to overcome this limitation. We provide with the analytic expressions of its constitutive parameters as functions of temperature. A detailed analysis of the experimental steady-state of deformation in stage I allows for a validation of the model. The role of secondary systems is discussed in view of the restrictions of the model validity to single slip loading cases.

II. MODELING OF Si CRYSTALS

A. Constitutive equations

Plastic deformation of silicon is assumed to proceed solely by motion and multiplication of dislocations on their slip planes. Deformation by twinning or non-Schmid effects such as climb are excluded from our discussion, for obvious reasons of simplicity. The total dislocation density \( \rho_1 \) on a slip system \( \alpha \) is assumed to be composed of mobile segments carrying plastic flow and of immobile ones trapped in dipolar or multipolar structures, of respective densities \( \rho_m^{(\alpha)} \) and \( \rho_i^{(\alpha)} \). It follows \( \rho_1^{(\alpha)} = \rho_m^{(\alpha)} + \rho_i^{(\alpha)} \). Orowan’s law \(^{20}\) bridges the gap between the microstructural variable \( \rho_m^{(\alpha)} \) and the macroscopic plastic strain rate \( \dot{\gamma}_p^{(\alpha)} \) and reads

\[
\dot{\gamma}_p^{(\alpha)} = \rho_m^{(\alpha)} \dot{b} v^{(\alpha)},
\]

(1)

where \( \dot{b} = 3.84 \times 10^{-10} \) m is the magnitude of the Burgers vector and \( v^{(\alpha)} \) the mean velocity of moving dislocations. It has been experimentally observed for isolated dislocations to vary linearly with the effective resolved shear stress \( \tau_{\text{eff}}^{(\alpha)} \) and to depend strongly on the temperature as \(^{21}\)

\[
v^{(\alpha)} = v_0 \left( \frac{\tau_{\text{eff}}^{(\alpha)}}{\tau_0} \right)^m \exp \left( - \frac{U}{k_B T} \right),
\]

(2)

with \( \tau_0 = 1 \) MPa, \( m = 1 \), and \( k_B = 8.617 \times 10^{-5} \) eV K\(^{-1}\) Boltzmann’s constant. The relevant values of the velocity prefactor \( v_0 \) and the activation energy \( U \) for dislocation motion depend on the rate-controlling dislocation character. They will be introduced for each constitutive model. We consider in this work intrinsic crystals only, so dopants and other impurities do not affect the activation energy.

The flow stress \( \tau^{(\alpha)} \) is assumed to equal the internal stress required to overcome short-range obstacles if present \( \tau_i^{(\alpha)} \) supplemented by the internal long-range elastic stress \( \tau_{\text{el}}^{(\alpha)} \) generated by mobile dislocations, and the effective stress \( \tau_{\text{eff}}^{(\alpha)} \) necessary for setting dislocations into motion,

\[
\tau^{(\alpha)} = \tau_i^{(\alpha)} + \tau_{\text{el}}^{(\alpha)} + \tau_{\text{eff}}^{(\alpha)}.
\]

(3)

The effective stress is defined by Eq. (4),

\[
\tau_{\text{eff}}^{(\alpha)} = \langle \tau^{(\alpha)} \rangle - \tau_i^{(\alpha)} - \tau_{\text{el}}^{(\alpha)},
\]

(4)

where \( \langle x \rangle = x \) if \( x > 0 \) and \( 0 \) otherwise.

1. AH model

The AH model aims at describing the yield region only. It suggests a generation term for mobile dislocations based on empirical data from germanium crystals \(^{22}\) and reminded in Eq. (5),

\[
\rho_m^{(\alpha)} = K \frac{\tau_{\text{eff}}^{(\alpha)} v^{(\alpha)}}{b},
\]

(5)

It assumes a characteristic linear dependency of generation on the effective stress \( \tau_{\text{eff}}^{(\alpha)} \), using a prefactor \( K \) constant at given loading conditions. All dislocations are assumed mobile, yielding \( \rho_i^{(\alpha)} = 0 \). The classical AH model neglects short-range interactions \( (\tau_i^{(\alpha)} = 0) \) and the influence of secondary dislocations both on dislocation generation and on the internal stress. The long-range internal stress is given by Eq. (6),

\[
\tau_i^{(\alpha)} = \mu b A \sqrt{\rho_m^{(\alpha)}},
\]

(6)

where \( A \) is a prefactor usually found to vary between 0.1 and 1.\(^{5,11,15}\)

Dislocation loops in the yield region exhibit a characteristic hexagonal shape made up of screw and 60° segments.\(^{22,23\)} The former are the slowest and limit the expansion rate of the loops. The dislocation motion parameters for the AH model are therefore \( v_0 = 3.5 \times 10^4 \) m s\(^{-1}\) and \( U = 2.35 \) eV.\(^{21}\)

2. Extended model

The extended model introduced in this work adds one internal variable to the AH model on each slip system, namely, the density of immobile dislocations \( \rho_i^{(\alpha)} \). Further improvements to the original model consist in the addition of short-range internal stresses and the presence of latent hardening coming both from long-range and short-range elastic interactions.

The dislocation densities are evolving following the net result of their generation, storage, and annihilation. In the present work, annihilation of stored dislocations is neglected for the sake of simplicity. We assume in addition that mobile dislocation segments belonging to the same slip system and gliding on parallel planes can trap each other and form dipolar structures. A mobile dislocation on a slip system \( \alpha \) crosses during the time \( dt \) a distance \( v^{(\alpha)} dt \). An effective capture radius \( r_c \) is defined for the storage of a mobile dislocation (see Fig. 1).\(^{24}\) Given a density \( \rho_m^{(\alpha)} \) of mobile dislocations on parallel planes, the amount of potential dipole formation events is \( \rho_m^{(\alpha)} 2 \pi r_c v^{(\alpha)} dt \). The rate of dipole formation on system \( \alpha \) is then \( \rho_m^{(\alpha)} (2 \pi r_c \rho_m^{(\alpha)}) \), equal to the rate of immobilization of mobile dislocations. The resulting evolution law for the density of mobile dislocations reads
The influence of the diagonal coefficients $A_{\alpha\alpha}$ will be discussed later on, the value found by dislocation dynamics simulations\cite{25} being higher than the 0.125 mentioned in Table I. The internal stress $\tau_{\alpha}^{p}$ comes from short-range interactions and emanates from the total dislocation densities.\cite{26} Its expression is given by Eq. (10),

$$\tau_{\alpha}^{p} = \mu b \sum_{\beta} A_{\alpha\beta} \rho_{m}^{\beta}.$$  

The coefficients $a_{\alpha\beta}$ are taken from latent hardening experiments on germanium crystals.\cite{25} Note that the diagonal effective self-interaction coefficient $a_{\alpha\alpha}$ is not null, as discussed in Refs. 28 and 29. The off-diagonal coefficients represent various hardening mechanisms coming from junction formation and collinear and coplanar interactions.

Observations indicate a predominance of edge or near edge dislocation segments in stage I, with the screws annihilating by cross-slip and the loops loosing their hexagonal shape under low effective stresses.\cite{17,30} The activation energy $U=2.2$ eV and the velocity prefactor $v_{0}=5 \times 10^{3}$ m s$^{-1}$ used by the extended model describe correctly the velocity of rate-dominating dislocations in stage I. These values are derived in Sec. V A. Table II summarizes the equations used by each constitutive model introduced in this section.

### B. Crystal plasticity framework

We use in this paper a crystal plasticity (CP) framework accounting for the discrete nature of plastic slip in crystals. This modeling approach gives more realistic results compared to a more standard isotropic formulation of plastic flow. The simultaneous activation of several slip systems and their mutual interactions are allowed by properly adapted constitutive laws.

The diamond cubic structure of silicon is similar to two embedded fcc structures translated by a quarter of diagonal from each other. Dislocation glide occurs on the closely spaced \{111\} planes (so-called glide set) and their associated \{110\} directions. This means that 12 primary slip systems are available for Si.\cite{32} The evolutions of dislocation densities on each of these slip systems are ruled by Eq. (5) or Eqs. (7) and (8), depending on the constitutive model considered. In a large-deformation formulation, the total displacement gradient $\mathbf{F}$ is decomposed multiplicatively into an elastic $\mathbf{F}^{e}$ and plastic part $\mathbf{F}^{p}$, as given in Eq. (11).\cite{33,34} Note that for simplicity, thermally induced deformations are not included in Eq. (11).\cite{35}

$$\mathbf{F} = \mathbf{F}^{e}\mathbf{F}^{p}.$$  

The former includes rigid-body motion and the elastic deformation of the lattice, while the latter represents the inelastic part of the deformation assumed to proceed by dislocation glide on the slip systems ($\alpha$), defined in the initial configuration by their normals $\mathbf{n}_{0}^{\alpha}$ and directions $\mathbf{s}_{0}^{\alpha}$. The plastic part of the velocity gradient is expressed as a function of the slip rates on the systems [Eq. (12)],

$$\mathbf{L}^{p} = \dot{\mathbf{F}}^{p}\mathbf{F}^{p-1} = \sum_{\alpha} \tau_{\alpha}^{p} \mathbf{s}_{0}^{\alpha} \otimes \mathbf{n}_{0}^{\alpha}.$$  

The resolved shear stress $\sigma^{(\alpha)}$ is defined as the work conjugate of the slip rate from the second Piola–Kirchhoff stress measure [Eq. (13)], in turn obtained assuming an hyperelastic material model [Eq. (14)].

$$\sigma^{(\alpha)} = \mathbf{S}^{\alpha} : \mathbf{F}^{eT} \mathbf{F}^{e}\mathbf{s}_{0}^{\alpha} \otimes \mathbf{n}_{0}^{\alpha},$$

$$\mathbf{S}^{\alpha} = \mathbf{L}^{e} : \mathbf{E}^{e} = \mathbf{L}^{e} \frac{1}{2} \left( \mathbf{F}^{eT} \mathbf{F}^{e} - \mathbf{I} \right).$$

The fourth-order stiffness tensor of silicon $\mathbf{L}$ is expressed with the help of its thermally dependent coefficients.\cite{36}

The constitutive models are implemented into a crystal plasticity routine as a user-defined material model (VUMAT) in ABAQUS/EXPLICIT. This finite element package requires the

### TABLE I. Interaction coefficients of the extended model. $A_{\alpha\beta}$: long-range (Ref. 25); $a_{\alpha\beta}$: short-range interactions (Ref. 27).

<table>
<thead>
<tr>
<th>Interaction</th>
<th>Self</th>
<th>Coplanar</th>
<th>Collinear</th>
<th>Hirth locks</th>
<th>Lomer locks</th>
<th>Glissile junction</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{\alpha\beta}$</td>
<td>(1/8)</td>
<td>1/16</td>
<td>1/20</td>
<td>1/12</td>
<td>1/12</td>
<td>1/12</td>
</tr>
<tr>
<td>$a_{\alpha\beta}$</td>
<td>0.09</td>
<td>0.09</td>
<td>0.41</td>
<td>0.06</td>
<td>0.12</td>
<td>0.12</td>
</tr>
</tbody>
</table>
TABLE II. Equations of the constitutive models considered in this work.

<table>
<thead>
<tr>
<th>Model</th>
<th>AH extended</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_m$</td>
<td>$\frac{K f_{\text{eff}} f_p}{b f_{\text{eff}} f_p}$</td>
</tr>
<tr>
<td>$\dot{\rho}_b$</td>
<td>0</td>
</tr>
<tr>
<td>$\dot{\tau}_p$</td>
<td>$\mu b \dot{\rho}_m \bar{p}_m^{\text{eff}}$</td>
</tr>
<tr>
<td>$\dot{\tau}_f$</td>
<td>0</td>
</tr>
</tbody>
</table>

update of the Cauchy stress tensor expressed in the corotational system at the end of each time increment, and care must be taken to keep track of the material rotation due to plastic shearing. More details about the implementation can be found in Ref. 38. The use of a CP framework in a finite element software is referred to as the CP-FEM approach in the following. Note that any of the two constitutive models introduced previously can indifferently be implemented in such a framework.

III. UNIAXIAL TENSILE TESTING OF SI MONOCRYSTALS

The simulations performed in this work aim at identifying model parameters using uniaxial tensile test data.

A. Experimental data

The experimental data used here are taken from the extensive work of Yonenaga et al.,14,15 who deformed float-zone (FZ) silicon monocrystals uniaxially in tension along the $[123]$ crystallographic axis. The tensile specimen were of rectangular cross section and had gauge dimensions of 2 $\times$ 3 $\times$ 30 mm. More details about sample preparation is given in Ref. 14. This paper concentrates on the effects of temperature only, from 1073 to 1223 K by 50 K increments. A constant unidirectional velocity is applied at one end of the structure while the other is kept fixed. The output Cauchy stress component along the tensile direction is averaged over the 12 central elements and sent to the optimization software for comparison with the experimental data.

B. Finite element model

A 3D monocrystalline tensile specimen similar to the ones used in experiments is created and meshed using 408 C3D8R solid elements of reduced integration (Fig. 3). The mesh size has been checked not to influence the results. The material behavior of the elements is defined by the VUMAT and the initial $[123]$ crystallographic orientation of the monocrystal relative to the tensile axis is defined in the internal variables.

FIG. 3. FE mesh used for analysis. Dark grayed elements: silicon tensile specimen. The 12 central elements used for output averaging are shown in white. Light gray elements: tensile apparatus.

C. Scalar formulation

The results obtained by CP-FEM will be compared to the ones provided by a classical scalar formulation when the constitutive model of Alexander and Haasen is chosen.5,11,15 The scalar approach is traditionally used to simulate uniaxial testing of monocrystals oriented for single glide. It assumes small deformations and the total shear strain rate is additively decomposed into an elastic and plastic parts: $\dot{\gamma} = \dot{\gamma}_p + \dot{\gamma}_f$. Since only one system is considered active the superscripts $(a)$ are not used. The resolved shear stress $\tau$ is obtained by integration of the elastic part of the shear strain rate, using an effective isotropic elastic shear modulus $\mu^e$ [Eq. (15), also called the machine equation],

$$\dot{\tau} = \mu^e (\gamma - \gamma_f).$$

(15)

It accounts for the combined stiffness of the sample and tensile apparatus and is found by calculating the initial slope of the experimental stress-strain curves. The scalar formulation...
assumes a constant shear strain rate acting on the silicon sample $\dot{\gamma}$.

**IV. ANALYSIS USING THE AH MODEL**

The parameters $K$ and $A$ of the AH model are determined by best fit to the experimental data of Fig. 2. Simulated annealing, a stochastic optimization method, was systematically chosen to ensure a global minima.39

**A. Strain rate in the yield region**

The influence of the tensile apparatus is visible at low strains. It is the result of the experimental stress-strain results by an initial slope that is well below the actual Young’s modulus (or shear modulus) of the material. The shear strain rate acting on the silicon specimen during the initial linear loading in the reference conditions, $\dot{\gamma}_e = \dot{\gamma}/\mu_{Si} = 10^{-11}$ s$^{-1}$, is then several orders of magnitude lower than the announced value of $1.2 \times 10^{-4}$ s$^{-1}$.

At the upper yield point, the relation $\dot{\tau}=0$ or $\dot{\gamma}=\dot{\gamma}_p = \rho_m b \sigma$ holds, and we can assume that the internal stress is small compared to the applied stress: $\dot{\tau}_{\text{up}} \approx \tau_{\text{eff},\text{up}}$. Combining Eqs. (1), (2), and (15) gives

$$\dot{\gamma}_{\text{up}} = \rho_{m,\text{up}} b \sigma_0 \exp \left( -\frac{U}{k_BT} \right) \tau_{\text{up}}.$$  

Equation (16) can be used to calculate the resolved shear strain rate at the upper yield point given the upper yield stress and the measured dislocation density. Using the experimental data in the reference conditions $\rho_{m,\text{up}} \approx 1.5 \times 10^{11}$ m$^{-2}$ and $\tau_{\text{up}} \approx 30$ MPa, the shear strain rate at the upper yield point is found to be roughly $5 \times 10^{-4}$ s$^{-1}$. This value is of the same order of magnitude as the announced $1.2 \times 10^{-4}$ s$^{-1}$.

The discrepancy might come from an overestimation of the dislocation density in such a dynamical state.

These observations point toward a variable effective strain rate in the yield region due to the tensile apparatus. The output from the FE model confirms this discussion and indicates a higher shear strain rate during the yield drop, before its value stabilizes at $1.2 \times 10^{-4}$ s$^{-1}$ beyond the lower yield point as shown in Fig. 4. Such a phenomenon leads to a sharper yield drop than if a constant strain rate were applied throughout the yield region. In spite of this variable strain rate, the resolved shear strain in the following figures assumes a perfect proportionality between time and strain to facilitate the readability of the results.

**B. Parameter identification**

Figure 5 shows the results using CP-FEM or a scalar formulation. The sets of constitutive parameters are similar within 5%. This confirms the equivalence between both frameworks.

The dislocation multiplication prefactor $K$ might vary with temperature because dislocation multiplication at the onset of silicon plasticity is observed to proceed partly by cross slip of screw segments, a thermally activated process.40 On the other hand, the internal stress prefactor $A$ should not depend on the deformation conditions, as it represents long-range, athermal elastic stress fields. Setting it to a fixed value of 0.3 (Refs. 12 and 15) results in underestimated lower yield stresses and the high $A$ values found by best fit [see Table III(b)] translate additional hardening mechanisms at the lower yield point. The very high purity of the floating-zone silicon crystals used in the experiments14 rules out a possible locking of dislocations by impurities,21,41 so the additional internal stress ought to be dislocation induced. It has been shown elsewhere42 that the variations and magnitude of $A$ do not depend sensitively on the choice of dislocation multiplication model. This unphysical temperature dependency translates a shortcoming of the AH model assuming that all dislocations are mobile and indicates as experimentally observed16 that the flow stress at the lower yield point and beyond is not uniquely constituted of a long-range component. Figure 6 compares stress-strain curves obtained using the constant [Fig. 6(a)] or temperature-dependent [Fig. 6(b)] $K$ and $A$ parameters as given in Table III.

**V. EXTENDED MODEL**

We consider in this section the storage of mobile dislocations by dipole formation and the presence of dislocation sources on the secondary systems. The model parameters to identify are therefore $K$, $r_c$, and $A_{\beta\beta}$, whereas the internal
stress coefficients \((A_{\alpha\beta})_{\alpha+\beta}\) and \(a_{\alpha\beta}\) are already known and taken from Refs. 25 and 27 (see Sec. II). The initial mobile dislocation density on the primary system is set to \(\rho_{\text{m,0}}^{(\text{prim})} = 2 \times 10^4 \text{ m}^{-2}\) and to \(\rho_{\text{m,0}}^{(\text{sec})} = 10^6 \text{ m}^{-2}\) on each of the secondary systems. The results are not qualitatively changed by increasing \(\rho_{\text{m,0}}^{(\text{sec})}\) by one order of magnitude. The initial densities of immobile dislocations on all slip systems are null.

**A. Preliminary discussion**

1. **Velocity of edge dislocation segments**

   It is commonly observed that both \(\rho_{\text{m}}^*\) and \(\tau_{\text{eff}}^*\) reach steady-state values in stage I \((\rho_{\text{m}}^*\) and \(\tau_{\text{eff}}^*\))

   Experimental results obtained at temperatures from 983 to 1273 K (Refs. 14 and 16) give for \(\gamma = 1.2 \times 10^{-4} \text{ s}^{-1}\) at steady state,

   \[
   \tau_{\text{eff}}^* = 1.13 \times 10^3 \exp\left(\frac{0.72}{k_bT}\right).
   \]

   The applied strain rate being temperature independent, Eq. (1) implies that \(\rho_{\text{m}}^* \propto \exp[(U-0.72)/k_bT]\) with \(U\) activation energy for dislocation motion. Experimental data 

   are very well fitted by Eq. (18),

   \[
   \rho_{\text{m}}^* = 5.93 \times 10^4 \exp\left(\frac{1.48}{k_bT}\right),
   \]

   confirming that the activation energy \(U\) for edge dislocation segments is closer to 2.2 eV than 2.35 eV during stage I, as argued in Sec. II A 2. The velocity prefactor \(v_0\) can be determined by two means, using Orowan’s law or a geometrical argument. A purely geometrical approach consists in approximating a 60° dislocation by a screw and an edge segments and obtaining their respective velocities by projection of the velocity vector. For the edge segment it gives \(v_0 = 5 \times 10^3 \text{ m s}^{-1}\). This simple model is validated by experimental data. The application of Eq. (1) in steady-state conditions gives

<table>
<thead>
<tr>
<th>Parameter</th>
<th>1073 K</th>
<th>1123 K</th>
<th>1173 K</th>
<th>1223 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>(K) ((10^4 \text{ N m}^{-1}))</td>
<td>3.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(A)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\rho_{\text{m}}^*) ((10^4 \text{ m}^{-2}))</td>
<td>2.5</td>
<td>3.4</td>
<td>3.8</td>
<td>7.4</td>
</tr>
<tr>
<td>(A)</td>
<td>0.88</td>
<td>0.78</td>
<td>0.63</td>
<td>0.58</td>
</tr>
</tbody>
</table>

**TABLE III. Best fitted parameters of the AH model.**

\(\gamma\), \(\tau_{\text{eff}}\), and \(v_0\) are already known and taken from Refs. 25 and 27 (see Sec. II). The initial mobile dislocation density on the primary system is set to \(\rho_{\text{m,0}}^{(\text{prim})} = 2 \times 10^4 \text{ m}^{-2}\) and to \(\rho_{\text{m,0}}^{(\text{sec})} = 10^6 \text{ m}^{-2}\) on each of the secondary systems. The results are not qualitatively changed by increasing \(\rho_{\text{m,0}}^{(\text{sec})}\) by one order of magnitude. The initial densities of immobile dislocations on all slip systems are null.

2. **Relations between constitutive parameters**

   Assuming the extended model correctly describes the dislocation evolution in silicon, Eq. (7) yields for \(\dot{\rho}_{\text{m}} = 0\),

   \[
   \rho_{\text{m}}^* = \frac{K\tau_{\text{eff}}^*}{2r_c}.
   \]

   It follows from the experimental data,

   \[
   \frac{\rho_{\text{m}}^*}{\tau_{\text{eff}}^*} = \frac{K}{2r_c} = 52 \exp\left(\frac{0.76}{k_bT}\right).
   \]

   The combined use of Orowan’s law and Eq. (21) at the steady state of deformation yields

   \[
   \rho_{\text{m}}^* \propto \frac{K}{r_c} \exp\left(\frac{U}{k_bT}\right).
   \]

   It can similarly be found that \((\tau_{\text{eff}}^*)^2 \propto (r_c/K) \exp(U/k_bT)\). This shows that the steady state of deformation predicted by the extended model is entirely defined by the ratio \(K/r_c\). Assuming the steady state of deformation and neglecting the dislocations on the secondary slip systems in stage I, the flow stress evolution reads

   \[
   \dot{\tau} = \dot{\tau}_1 = \frac{\mu b}{2} \sqrt{\frac{\dot{\gamma}}{\rho_{\text{m}}}} \frac{\rho_{\text{m}}}{\rho_{\text{m}}},
   \]

   with \(\rho_{\text{m}} = K\tau_{\text{eff}}^* \gamma/b\) and \(\rho_{\text{m}} = \rho_{\text{m}}^0 + K\tau_{\text{eff}}^*(\gamma - \gamma_0)/b\) with \(\rho_{\text{m}}^0\) total dislocation density at \(\gamma_0\). Taking \(\gamma_0\) large enough so we can assume \(\rho_{\text{m}} \Delta t \ll \rho_{\text{m}}^0\) and noting the athermal nature of the hardening rate in stage I \([(\partial \rho_{\text{m}}/\partial T)(d\rho_{\text{m}}/d\rho_{\text{m}}) \approx 0]\) gives

   \[
   K \propto \frac{1}{(\tau_{\text{eff}}^*)^2}.
   \]

   This second relationship leads to the complete description of the variations in \(K\) and \(r_c\) with temperature,

   \[
   \left\{ \begin{array}{l}
   K \propto \exp\left(-\frac{0.72}{k_bT}\right) \\
   r_c \propto \exp\left(-\frac{1.48}{k_bT}\right).
   \end{array} \right.
   \]
pendent parameters only: the self-interaction coefficient for long-range elastic interactions $A_{\beta \beta}$ and either $K$ or $r_c$ and the temperature dependency of the two last ones being readily known.

A first limitation of the extended model is the absence of dependency of the constitutive parameters on the strain rate. It is experimentally observed that doubling the strain rate results in a significantly different mechanical response of silicon monocrystals.\textsuperscript{5,14} Considering solely temperature-dependent parameters is an approximation made for the sake of simplicity. The large variations in the strain rate in the yield region (Fig. 4) are bound to influence the values of $K$ and $r_c$ mentioned in the following. Its second limitation comes from the assimilation of all dislocations to edge ones, resulting in a possibly poor representation of the yield region dominated by screw and 60° segments.

### B. Parameters identification

The constitutive parameters obtained by individual best fits are given in Table IV, where the relations derived previously are ignored. The self-interaction coefficient $A_{\beta \beta}$ is fixed in this first approach. Both $K$ and $r_c$ are seen to increase with temperature. One can note that the ratio $K/2r_c$ is one order of magnitude lower than the requirement of Eq. (21).

The activation energies for $r_c$ and $K$ are now set dependent following Eqs. (21) and (25). Long-range stresses from self-interactions are modulated by the free parameter $A_{\beta \beta}$. The sum of the cost functions for all four experimental data is then minimized for the following values:

\[
\begin{align*}
A_{\beta \beta} &= 0.21 \\
K(T) &= 7.6 \times 10^{-1} \exp \left( -\frac{0.72}{k_b T} \right) \\
r_c(T) &= 7.2 \times 10^{-3} \exp \left( -\frac{1.48}{k_b T} \right),
\end{align*}
\]

where $K$ is expressed in m N\(^{-1}\) and $r_c$ in meters. The resulting simulated stress-strain curves are plotted in Fig. 7. Note that although the parameters have been identified using the yield region only, the simulated mechanical behavior is in very good agreement with the experimental one throughout stage I of deformation. This confirms that the hardening mechanisms assumed in Eqs. (7) and (8) remain valid during stage I. The model predicts an additional softening when secondary systems are activated and is consequently not appropriate for stage II hardening. This could be foreseen by the absence of dislocation storage on the forest in Eqs. (7) and (8). The simulated stress-strain curves become more accurate as temperature is increased.

### C. Analysis of the model outputs

#### 1. Verification of the best fitted parameters

The steady state of the effective stress and of mobile dislocation density are observed in simulations as shown in Fig. 8. Enforcing Eq. (21) imposes constraints on $\rho_u^e$ and $\tau_u^e$ that can be overcome by increasing the internal stress if $A_{\beta \beta} = 0.125$ is taken as the base case. $A_{\beta \beta} = 0.21$ allows for full compliance of $K$ and $r_c$ to this empirical relation without impacting the accuracy of the simulated stress-strain behavior. An excellent agreement is observed between the experimental and predicted steady-state variables. This $A_{\beta \beta}$ value is of the same order of magnitude as the 0.3 usually mentioned in the literature.\textsuperscript{11,12,15}

The numerical values of $K$ given by Eq. (26) are very close to the ones introduced in Table IV. This was expected since this parameter determines the magnitude of the upper yield point.

Observations of thin foils from silicon samples deformed at the end of stage I at 1073 K yield for the maximum value of the dipole half width $r_c^{\text{max}} = 6 \times 10^{-7}$ m.\textsuperscript{17} $r_c$ is an effective dipole half width and can be approximated via the average square dipole width,\textsuperscript{44}

\[
r_c = \sqrt{(e-1)r_c^{\text{max}}r_u},
\]

where $r_u$ is the critical half width for dipole annihilation, typically a couple of Burgers vectors.\textsuperscript{45} Taking at 1073 K $r_u = 10^{-9}$ m gives $r_c = 3.2 \times 10^{-8}$ m, one order of magnitude larger than the result given by Eq. (26) but comparable to the individual best fits (Table IV). The capture radius found by simultaneous fit of the extended model to experimental data is consequently much lower than its empirical values when the correct steady state of deformation is imposed through Eqs. (21) and (25). This results in an overestimation of the ratio $\rho_m/\rho_i$ (see below).

#### 2. Influence of secondary slip systems

No multiplication or storage of dislocations from mutual interaction between slip systems is introduced in the constitutive model. The only way for secondary dislocations to be generated in simulations is by overcoming the critical resolved shear stress for setting them into motion and fulfilling the relation $|\tau_i^{(a)}| \geq \tau_i^{(a)} + \tau_u^{(a)}$. This condition is realized mainly before the lower yield point. The secondary dislocation density continues to grow beyond but at a slow pace, remaining two to three orders of magnitude below the primary density during stage I (see Fig. 9). It follows that vir-
tually all dislocations are present on the primary slip system throughout deformation. Secondary systems become active as the lattice rotates with deformation around \( \gamma = 30\% \). The constitutive model loses its validity at this point.

It is experimentally observed at 1073 K that 10% of the total dislocation density is on secondary systems at the lower yield point, this fraction diminishing as temperature is heightened.\(^{14}\) The extended model cannot represent this phenomena. Adding a storage term proportional to the mean free path of dislocations on their glide plane\(^{8,9}\) could improve this point, indicating that dislocation multiplication and storage mechanisms on the forest trees are active in silicon crystals even at low densities. The additional hardening provided by such a small percentage of forest dislocations could also explain the discrepancy between the simulated and experimental flow stresses at lower temperatures (Fig. 7).

Dislocations on the secondary slip systems can safely be disregarded when using such a constitutive model in single glide conditions only. The absence of dislocation storage on the forest actually prevents any appearance of stage II hardening in purely uniaxial tensile simulations. The model introduced in this work can therefore be used in combination with a scalar framework.

### 3. Mechanical state at the lower yield point

Comparison of the model outputs with additional experimental data\(^{10}\) shows that it predicts successfully the effective resolved shear stress at the lower yield point and the internal stress coming from short-range interactions \( \tau_e \). The model parameters nonetheless overestimate the fraction of mobile dislocations \( \langle \rho_m/\rho \rangle_{\text{exp}} \), 75%–90% depending on temperature. Yonenaga\(^{16}\) reported in the reference conditions fractions of 35%–40% in silicon, still far from the simulated quantities. This discrepancy stems directly from the underestimation of the effective capture radius underlined above.

A direct consequence of these remarks is that the extended model based on the empirical generation law suggested by Alexander and Haasen cannot guarantee full agreement between experimental data and simulations. Increasing \( r_c \) by one order of magnitude to bring its value closer to physical ones and to reduce \( \langle \rho_m/\rho \rangle_{\text{exp}} \), results, if Eq. (21) is to be strictly enforced, in a multiplication prefactor too high to correctly represent any yield phenomena. The multiplication law of Alexander and Haasen cannot yield accurately mobile dislocation densities and the steady state of deformation simultaneously, if the experimental stress-strain curves are to be correctly represented.

### VI. CONCLUSION

Using a scalar formulation for modeling the mechanical behavior of silicon monocrystals deformed in single glide with the help of the machine equation is equivalent to the adoption of a crystal plasticity framework into a finite element code. The influence of the tensile equipment is then no longer translated by an effective shear modulus but by the introduction of elastic elements bounding the tensile specimen. The advantage of the latter approach is to explore the eventual activation of secondary systems upon uniaxial loading. A scalar formulation is indeed not appropriate when complex, 3D loadings are applied.

The traditional model of Alexander and Haasen assumes all dislocations mobile in the yield region and predicts an effective stress at the lower yield point roughly one-third of the applied stress. We have shown that in order to correctly describe the mechanical behavior of silicon crystals, its parameters must vary significantly with temperature. In particular, the variations in the internal stress prefactor are not physically acceptable as it represents athermal long-range elastic stress fields. The introduction of a density of immobile dislocations trapped in dipolar or multipolar structures, as well as of short-range elastic stresses and latent hardening mechanisms, allows for correcting this shortcoming and leads to good agreement with experiments.

Observations of the steady state of deformation beyond the lower yield point in different loading conditions provide with the expression of the velocity of edge dislocations. Two equations can be derived, linking the parameters of the constitutive model introduced in this work. The dislocation generation parameter \( K \) from the AH model and the effective capture radius for storage of dislocations \( r_c \) are then dependent from each other. The steady state of deformation in stage I is completely defined by their ratio, the long-range...
self-interaction prefactor $A_{BB}$ allowing good fits between simulations and experimental stress-strain curves.

The extended model predicts lower flow stresses and higher fractions of mobile dislocations than experimentally found, but performs better as temperature increases. This is shown to come primarily from the absence of generation and storage terms from the forest in the dislocation evolution laws, and secondly because of the underestimation of the $r_c$ parameter at lower temperatures. The model is unable to represent stage II of hardening for the same reasons. It follows that the constitutive equations introduced in this work can be used in a simple scalar or Von Mises formulation of plastic flow considering one slip system only without a loss of accuracy, provided large strains are allowed for.

Finally, we have underlined the inability of the model to predict simultaneously a low fraction of mobile dislocations at and beyond the lower yield point and the values of the steady-state mobile dislocation density and effective stress. Accounting for the strain-rate dependency of the constitutive parameters might improve the accuracy of our model and allow for its application in a broad range of loading conditions. The current parameters predict upper yield stresses accurate within 15\% at 1173 K and strain rates of $6 \times 10^{-5}$ and $6 \times 10^{-4}$ s$^{-1}$, which is rather satisfying. The temperatures at which the constitutive equations can be used are limited to the range where dislocation motion follows the double kink mechanism. Diffusion processes observed above 1300 K (Refs. 46 and 47) are an example of limitation to the applicability of the constitutive model introduced in this work. A complete constitutive model valid into stage II of deformation will be introduced in a forthcoming paper.

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