Details about how to include non-Schmid effects on kMC simulations

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Kink pairs can only form on {110}-type planes. However, the maximum resolved shear stress (MRSS) plane may not coincide with one of these {110} planes. For the derivations that will be undertaken here, the following notation is assumed:

- $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ is the angle between the positive x axis and the {110} plane where kink pairs are to be nucleated.

- $-\frac{\pi}{2} < \theta_{\text{MRSS}} < \frac{\pi}{2}$ is the angle between the positive x axis and the MRSS plane.

- $-\frac{\pi}{6} < \chi < \frac{\pi}{6}$ is the angle between the {110} plane and the MRSS plane.

With these definitions, the angles θ and χ can be related via the expression:

$$\theta = \theta_{\text{MRSS}} - \chi \tag{1}$$

According to Schmid law, the RSS for a general plane can be calculated as:

$$\sigma_{\text{RSS}} = \boldsymbol{t} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{n} \tag{2}$$

where $\boldsymbol{\sigma}$ is the stress tensor, and $\boldsymbol{t} = \boldsymbol{b}/\|\boldsymbol{b}\|$ and $\boldsymbol{n}$ are unit vectors representing the slip direction and slip plane normal. For a screw dislocation in the standard reference system ($\boldsymbol{b} \equiv [0\ 0\ b]$, $\boldsymbol{t} \equiv [0\ 0\ 1]$, $\boldsymbol{n} \equiv [-\sin\theta\ \ \cos\theta\ 0]$), expanding eq. 2 results in:

$$\sigma_{\text{RSS}} = (0\ 0\ 1) \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} n_x \\ n_y \\ 0 \end{pmatrix} = \sigma_{xz} n_x + \sigma_{yz} n_y = -\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta \tag{3}$$

1 Finding the MRSS plane from a general stress tensor

To find the MRSS plane, we differentiate the above expression w.r.t. θ:

$$\frac{\partial \sigma_{\text{RSS}}}{\partial \theta} = -\sigma_{xz}\cos\theta - \sigma_{yz}\sin\theta$$

The condition to have a maximum is:

$$\frac{\partial \sigma_{\text{RSS}}}{\partial \theta} = 0 \tag{4}$$

$$\frac{\partial^2 \sigma_{\text{RSS}}}{\partial \theta^2} < 0 \tag{5}$$

Enforcing eq. 4, we arrive at:

$$\tan\theta = -\frac{\sigma_{xz}}{\sigma_{yz}}$$

i.e.:

$$\boxed{\theta_{\text{MRSS}} = \tan^{-1}\left(-\frac{\sigma_{xz}}{\sigma_{yz}}\right)} \tag{6}$$

The above expression satisfies the necessary limits that if $\sigma_{xz} = 0 \to \theta_{\text{MRSS}} = 0$ and if $\sigma_{xz} = 0 \to \theta_{\text{MRSS}} = \frac{\pi}{2}$ (θ_{MRSS} is measured w.r.t. the right x-axis). Equation 6 gives the MRSS plane from a general stress tensor in the frame of reference of the kMC code: $\boldsymbol{n}_{\text{MRSS}} \equiv [-\sin\theta_{\text{MRSS}} \;\; \cos\theta_{\text{MRSS}} \;\; 0]$. One can also enforce eq. 5 to ensure that $\boldsymbol{n}_{\text{MRSS}}$ corresponds to a maximum:

$$\begin{aligned} \frac{\partial^2 \sigma_{\text{RSS}}}{\partial \theta^2} &= \sigma_{xz}\sin\theta - \sigma_{yz}\cos\theta < 0 \\ \tan\theta_{\text{MRSS}} &< \frac{\sigma_{yz}}{\sigma_{xz}} \end{aligned}$$

2 Computing the angle between the MRSS plane and a given $\{110\}$ plane

Then, the angle χ can be obtained as the angle formed by the MRSS plane and the local $\{110\}$-type plane where kink pairs can nucleate (in general, there will be several of these). In other words:

$$\chi = \cos^{-1}\left(\boldsymbol{n}_{\{110\}} \cdot \boldsymbol{n}_{\text{MRSS}}\right) \tag{7}$$

This equation should be checked against eq. 1 for consistency.

In bcc metals, a deviation from eq. 2 is observed. Typically, this deviation is measured in terms of the critical stress as a function of the angle χ. This does not mean that the Peierls stress changes, it is simply a convention to measure non-Schmid behavior. In the literature, the non-Schmid law is generally expressed as:

$$\boxed{\sigma_c^\chi = \frac{a_1\sigma_P}{\cos\chi + a_2\cos(\chi + 60°)}} \tag{8}$$

where a_1 and a_2 are fitting constants. For the MEAM potential, $a_1 = 1.32$ and $a_2 = 0.64$ ($\sigma_P = 3200$ MPa). The above formula is symmetric about the limits of the $[-30° : +30°]$ interval, which means that the following relations have to be applied to eq. 7:

$$\text{positive semiplane} \begin{cases} \text{if} \quad 0° < \chi < 30° & \text{then} \quad \chi = \chi \\ \text{if} \quad 30° < \chi < 90° & \text{then} \quad \chi = 60° - \chi \\ \text{if} \quad 90° < \chi < 150° & \text{then} \quad \chi = \chi - 120° \\ \text{if} \quad 150° < \chi < 180° & \text{then} \quad \chi = 180° - \chi \end{cases}$$

$$\text{negative semiplane} \begin{cases} \text{if} \quad -30° < \chi < 0° & \text{then} \quad \chi = \chi \\ \text{if} \quad -90° < \chi < -30° & \text{then} \quad \chi = -60° - \chi \\ \text{if} \quad -150° < \chi < -90° & \text{then} \quad \chi = 120° + \chi \\ \text{if} \quad -180° < \chi < -150° & \text{then} \quad \chi = -180° - \chi \end{cases}$$

3 Computing the non-Schmid resolved shear stress

Now, the RSS is obtained by projection as:

$$\sigma_{RSS} = -\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta \tag{9}$$

To compute the non-dimensional stress s used in the kMC code, we normalize by the *critical* stress σ_c^χ according to eq. 8:

$$s = \frac{\sigma_{RSS}}{\sigma_c^\chi} = \frac{-\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta}{a_1\sigma_P}\left(\cos\chi + a_2\cos(\chi + 60°)\right) \tag{10}$$

where, again, $\theta = \theta_{\text{MRSS}} - \chi$. To check the validity of expression 10, we consider the following scenarios in order of complexity:

(i) $\theta = \theta_{\mathrm{MRSS}} = \chi = 0$: $s = \frac{\sigma_{yz}}{\sigma_P}$

(ii) $\theta = 0$, $\theta_{\mathrm{MRSS}} = \chi$: $s = \sigma_{yz} \left(\cos\chi + a_2 \cos(\chi + 60°) \right) / a_1 \sigma_P$

(iii) $\theta \neq 0$, $\theta_{\mathrm{MRSS}} = 0$, $\chi = \theta$: $s = \left(-\sigma_{xz} \sin\theta + \sigma_{yz} \cos\theta \right) \left(\cos\chi + a_2 \cos(\chi + 60°) \right) / a_1 \sigma_P$

Case (ii) is the most resorted-to scenario in books and scientific papers. The resulting expression:

$$s = \frac{\sigma_{yz}(\cos\chi + a_2 \cos(\chi + 60°))}{a_1 \sigma_P} = \frac{\sigma_{yz}}{\sigma_c^{\chi}} \tag{11}$$

is interpreted as if σ_c^{χ} was a χ-dependent Peierls stress, when in reality it simply contains the standard (Schmid) cos term from the projected stress tensor plus a nonlinear correction.

Therefore, eq. 10 is the correct one when non-Schmid effects are included and the one that should be used in the kMC code. In calculations, once the possible $\{110\}$ glide planes have been identified, the angles χ and θ are obtained and then s is calculated for each one of them as:

$$s(\theta, \chi) = \frac{\sigma_{\mathrm{RSS}}(\theta)}{\sigma_c^{\chi}(\chi)} \tag{12}$$