1 Inputs

The parameter s will be computed from the following inputs:

- $\boldsymbol{\sigma}$ - Local stress tensor. $\boldsymbol{\sigma}$ is defined in the global simulation coordinate system. The only significant components are σ_{xz} and σ_{yz}.
- $\boldsymbol{b} = (0, 0, b)^T$ - Burgers vector
- $\theta \in [0, 2\pi)$ - Angle of kink direction, measured from the positive x-axis of the simulation coordinate system. In the bcc system there are six possible kink directions: $\theta = \frac{\pi}{3}k \quad (k = 0 \ldots 5)$.

The unit normal of the kink plane is

$$\boldsymbol{n}_k = (-\sin\theta, \cos\theta, 0)^T \tag{1}$$

2 Schmid law

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

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

where $\boldsymbol{t} = \boldsymbol{b}/\left|\boldsymbol{b}\right| = (0, 0, 1)$ and $\boldsymbol{n}$ are unit vectors representing the slip direction and slip plane normal. Expanding Eq. 2 and using Eq. 1 results in:

$$\sigma_{\mathrm{RSS}}(\theta) = -\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta \tag{3}$$

3 Maximum resolved shear stress (MRSS)

The direction of maximum resolved shear stress is denoted by the angle θ_{MRSS} and can be computed from the stress tensor components:

$$\theta_{\mathrm{MRSS}} = \arctan\left(-\frac{\sigma_{xz}}{\sigma_{yz}}\right). \tag{4}$$

The value of the MRSS can also be computed from the components of the stress tensor as follows:

$$\sigma_{\mathrm{MRSS}} = \sqrt{\sigma_{xz}^2 + \sigma_{yz}^2} \tag{5}$$

PROOF: Insert Eq. 4 into Eq. 3:

$$
\begin{aligned}
\sigma_{\mathrm{MRSS}} &= \sigma_{\mathrm{RSS}}(\theta_{\mathrm{MRSS}}) && (6)\\
&= -\sigma_{xz}\sin\left[\arctan\left(-\frac{\sigma_{xz}}{\sigma_{yz}}\right)\right] + \sigma_{yz}\cos\left[\arctan\left(-\frac{\sigma_{xz}}{\sigma_{yz}}\right)\right] && (7)\\
&= \sigma_{xz}\cdot\frac{\sigma_{xz}}{\sigma_{yz}}/\sqrt{1+\frac{\sigma_{xz}^2}{\sigma_{yz}^2}} + \sigma_{yz}/\sqrt{1+\frac{\sigma_{xz}^2}{\sigma_{yz}^2}} && (8)\\
&= \sigma_{xz}^2/\sqrt{\sigma_{yz}^2+\sigma_{xz}^2} + \sigma_{yz}^2/\sqrt{\sigma_{yz}^2+\sigma_{xz}^2} && (9)\\
&= \sqrt{\sigma_{xz}^2+\sigma_{yz}^2} && (10)
\end{aligned}
$$

4 Critical shear stress

The direction of maximum resolved shear stress, θ_{MRSS}, and the kink direction, θ, form the angle χ:

$$\chi = \theta_{\mathrm{MRSS}} - \theta \tag{11}$$

We can imagine an experiment in which θ_{MRSS} is fixed and σ_{MRSS} is incremented in small steps until slip occurs on the kink plane given by θ. We call this critical value of σ_{MRSS} the *Critical Resolved Shear Stress* (CRSS) $\sigma_c(\chi)$. It depends on the angle χ between the kink plane and the MRSS plane. Furthermore, we can define a parameter

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

which measures the fraction of the critical stress reached at current level of stress. The condition $s(\chi) = 1$ means that the shear stress resolved on the direction $\theta_{\mathrm{MRSS}} = \theta + \chi$ reaches the critical level required to let the dislocation move in the glide direction θ.

The above discussion applies to both Schmid and non-Schmid behavior.

5 Critical stress and the Schmid law

In a material that follows Schmid's law, the CRSS $\sigma_c(\chi)$ exhibits a $1/\cos\chi$ dependence:

$$\sigma_c(\chi) = \frac{\sigma_P}{\cos\chi} \tag{13}$$

with σ_P being a material constant. We now have to show that this interpretation really corresponds to the classical formulation of Schmid's law (Eq. 3). Given that σ_P is the critical resolved stress that must be reached on the glide plane to trigger slip, then the actual resolved shear stress on the glide plane is $\sigma_{\mathrm{RSS}} = s \cdot \sigma_P$. We begin by inserting Eqs. 12 and 13:

$$
\begin{aligned}
\sigma_{\mathrm{RSS}} &= s(\chi) \cdot \sigma_P && (14)\\
&= \frac{\sigma_{\mathrm{MRSS}}}{\sigma_c(\chi)} \cdot \sigma_P && (15)\\
&= \frac{\sigma_{\mathrm{MRSS}}}{\sigma_P / \cos\chi} \cdot \sigma_P && (16)\\
&= \sigma_{\mathrm{MRSS}} \cos\chi && (17)\\
&= \sigma_{\mathrm{MRSS}} \cos(\theta_{\mathrm{MRSS}} - \theta) && (18)\\
&= \sigma_{\mathrm{MRSS}} \left[\sin\theta_{\mathrm{MRSS}} \sin\theta + \cos\theta_{\mathrm{MRSS}} \cos\theta\right] && (19)\\
&= \underbrace{\sigma_{\mathrm{MRSS}} \sin\theta_{\mathrm{MRSS}}}_{=-\sigma_{xz}} \sin\theta + \underbrace{\sigma_{\mathrm{MRSS}} \cos\theta_{\mathrm{MRSS}}}_{=\sigma_{yz}} \cos\theta && (20)\\
&= -\sigma_{xz} \sin\theta + \sigma_{yz} \cos\theta && (21)
\end{aligned}
$$

This is indeed identical to the Schmid law (Eq. 3). Note that we have shown the validity of definition (12) for arbitrary θ (and θ_{MRSS} or χ).

6 Implementation of non-Schmid corrections

For materials that exhibit non-Schmid effects, we have to modify the CRSS's dependence on χ given by Eq. 13. We use the following modified form to account for non-Schmid effects:

$$\sigma_c(\chi) = \sigma_P \frac{a_1}{\cos\chi + a_2 \cos(\chi + \frac{\pi}{3})}. \quad (22)$$

Computing the parameter s:

$$
\begin{aligned}
s(\theta, \chi) &= \frac{\sigma_{\mathrm{MRSS}}}{\sigma_c(\chi)} && (23)\\
&= \sigma_{\mathrm{MRSS}} \frac{\cos\chi + a_2 \cos(\chi + \frac{\pi}{3})}{\sigma_P a_1} && (24)\\
&= \sqrt{\sigma_{xz}^2 + \sigma_{yz}^2} \frac{\cos\chi + a_2 \cos(\chi + \frac{\pi}{3})}{\sigma_P a_1} && (25)
\end{aligned}
$$

with $\chi = \theta_{\mathrm{MRSS}} - \theta = \arctan\left(-\frac{\sigma_{xz}}{\sigma_{yz}}\right) - \theta$.

We finally show that the normal Schmid behavior can be retained by setting $a_1 = 1, a_2 = 0$:

$$s(\theta, \chi) = \sigma_{\mathrm{MRSS}} \frac{\cos\chi + a_2 \cos(\chi + \frac{\pi}{3})}{\sigma_P a_1} \quad (26)$$

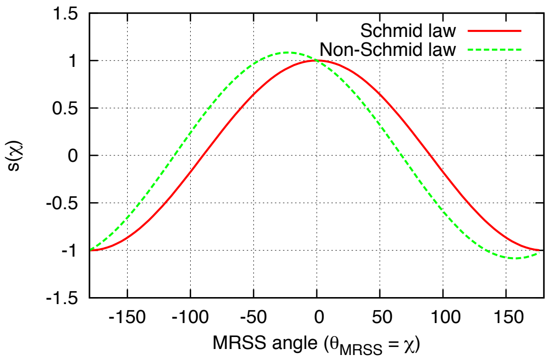
$$= \sigma_{\text{MRSS}} \frac{\cos\chi}{\sigma_P} \quad (27)$$

$$= \left[-\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta\right] / \sigma_P \quad (28)$$

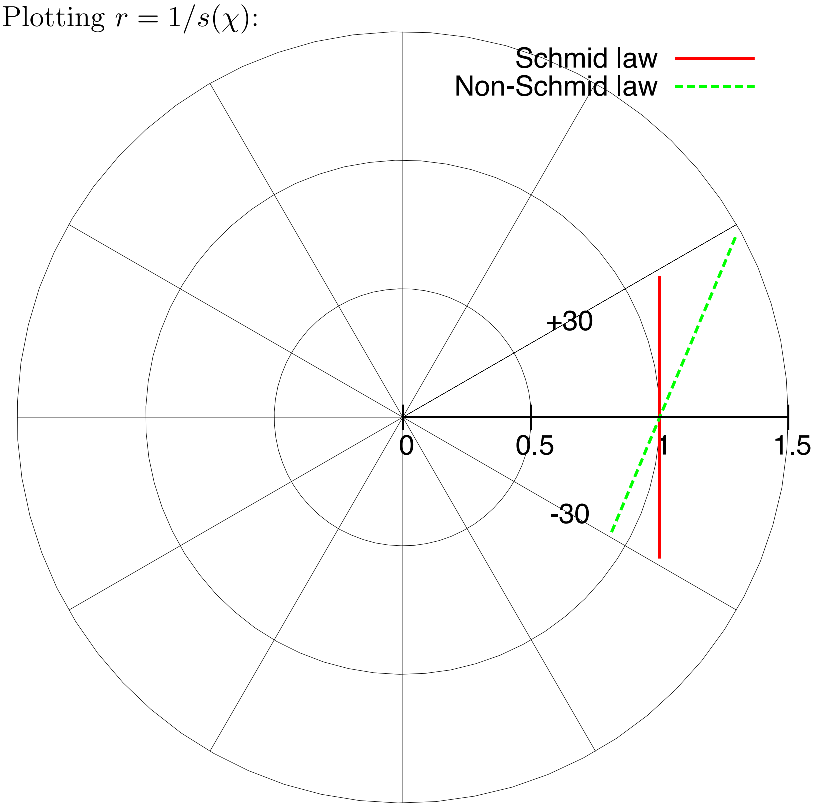
In the last step we re-used the derivations (17)-(21).

7 Numerical test 1

We consider the following scenario: $\theta = 0$, $\chi = \sigma_{\text{MRSS}} \in [0, 2\pi)$, $a_1 = 1.32$, $a_2 = 0.64$



Plotting $r = 1/s(\chi)$:



8 Numerical test 2

$\theta = -60$ degrees: