Supplementary information - Dislocation dynamics study of precipitate hardening in Al-Mg-Si alloys with input from experimental characterization

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1 Derivation of forces on the dislocation due to the precipitate

In this supplementary information we will show the full derivation of the forces used to implement precipitates into the dislocation dynamics code, as explained in section 2.1 in the main paper.

The equilibrium equation for elastic problem for a sphere in spherical coordinates is posed as follows

$$\frac{d}{dr}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2 u(r)\right)\right) = 0 \tag{1}$$

r being the radius and u the displacement field. With spherical symmetry u only depends on r. From this expression we want to calculate the force outside the elastic inclusion, assuming the inclusion is impenetrable by the dislocation.

Solving the equation above with the boundary conditions

$$u(R) = \quad c \tag{2}$$

$$u(\inf) = \quad 0 \tag{3}$$

where R is the radius of the precipitate, we get

$$u(r) = c\left(\frac{R}{r}\right)^2 \tag{4}$$

Once we have calculated the displacement field we have to obtain the stress and strain tensors. In this truly symmetric problem both tensors are given as follows

$$\begin{pmatrix} \sigma_{rr} & 0 & 0 \\ 0 & \sigma_{\theta\theta} & 0 \\ 0 & 0 & \sigma_{\phi\phi} \end{pmatrix}; \begin{pmatrix} \epsilon_{rr} & 0 & 0 \\ 0 & \epsilon_{\theta\theta} & 0 \\ 0 & 0 & \epsilon_{\phi\phi} \end{pmatrix} \tag{5}$$

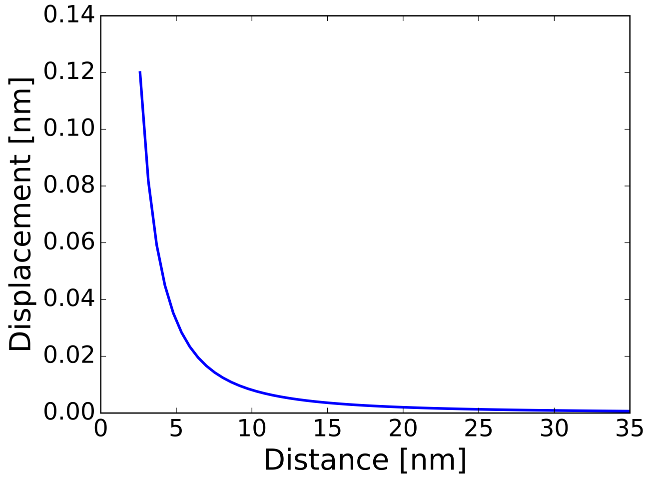

Figure S1: Displacement field around a spherical inclusion

Also, $\sigma_{\theta\theta} = \sigma_{\phi\phi}$ and $\epsilon_{\theta\theta} = \epsilon_{\phi\phi}$. For this case the strain components are given by the following relations

$$\epsilon_{rr} = \frac{du}{dr} \tag{6}$$
$$\epsilon_{\theta\theta} = \epsilon_{\phi\phi} = \frac{u}{r} \tag{7}$$

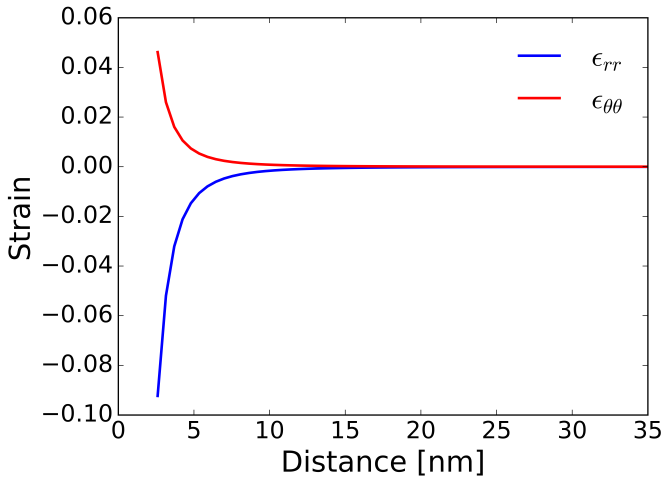

Figure S2: Strain field outside a spherical inclusion

And from the strains we obtain the stresses

$$\sigma_{rr} = \frac{E}{(1+\nu)(1-2\nu)}\left((1-\nu)\,\epsilon_{rr} - 2\nu\epsilon_{\theta\theta}\right) \tag{8}$$

$$\sigma_{\theta\theta} = \sigma_{\phi\phi} = \frac{E}{(1+\nu)(1-2\nu)}(\epsilon_{\theta\theta} + \nu\epsilon_{rr}) \tag{9}$$

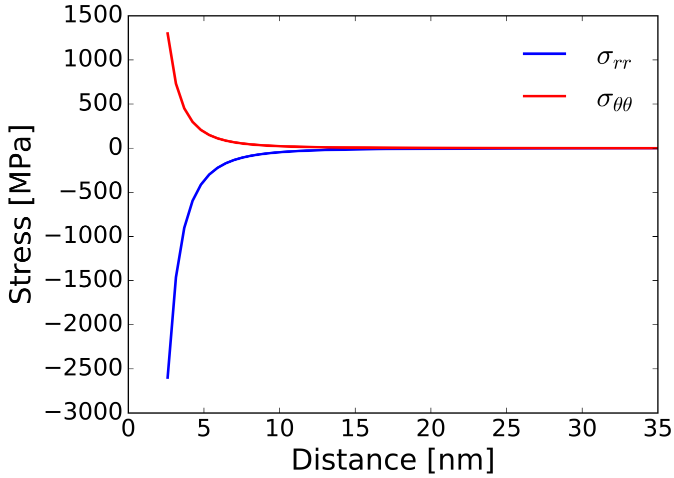

Figure S3: Stress field outside a spherical inclusion

For the stresses outside the precipitate we get

$$\sigma_{rr} = -\frac{2ER^2c}{r^3(\nu+1)} \tag{10}$$

$$\sigma_{\theta\theta} = \frac{ER^2c}{r^3(\nu+1)} \tag{11}$$

Once we have the stress tensor we solve for the forces on a dislocation segment through the Peach-Koeler expression

$$\overrightarrow{df} = \tilde{\sigma}\,\overrightarrow{b} \times \overrightarrow{t}\,dz \tag{12}$$

We are going to define a new basis such that the $\overrightarrow{k}$ direction is given by $\parallel \overrightarrow{r_2} - \overrightarrow{r_1} \parallel$ and the segment is on the plane defined by $\overrightarrow{k} \times \overrightarrow{i}$. For simplicity the basis of the stress tensor will be changed from spherical coordinates to cartesian. The basis change matrix is given by

$$B = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \end{pmatrix} \tag{13}$$

And the transformation itself $\tilde{\sigma_e} = \tilde{B}^T\tilde{\sigma_u}\tilde{B}$, where the subscript e stands for cartesian coordinates and

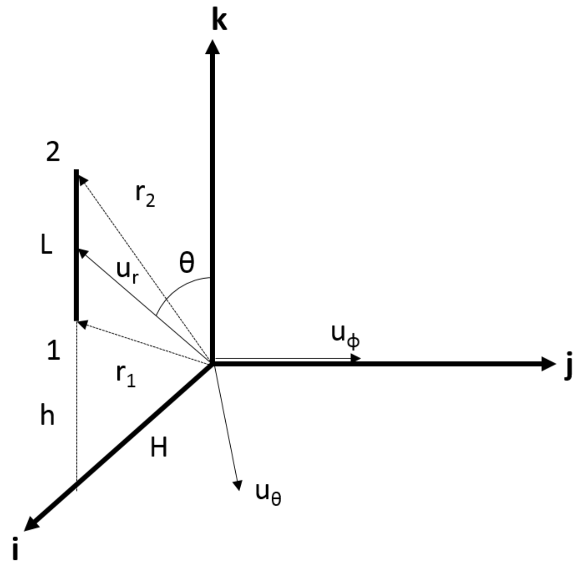

Figure S4: Coordinate system.

u for spherical coordinates, resulting then in

$$\tilde{\sigma_e} = \begin{pmatrix} \sigma\phi\phi & 0 & 0 \\ 0 & \sigma rr \sin^2\theta + \sigma_{\theta\theta}\cos^2\theta & \sigma rr \sin\theta\cos\theta + \sigma_{\theta\theta}\cos\theta\sin\theta \\ 0 & \sigma rr \sin\theta\cos\theta + \sigma_{\theta\theta}\cos\theta\sin\theta & \sigma rr \sin^2\theta + \sigma_{\theta\theta}\cos^2\theta \end{pmatrix} \tag{14}$$

And now resolving the Peach-Koeler expression

$$\overrightarrow{df} = \begin{pmatrix} b_2(\sigma_{rr} - \sigma_{\theta\theta})\sin^2\theta + b_2\sigma_{\theta\theta} + b_3(\sigma_{rr} - \sigma_{\theta\theta})\sin\theta\cos\theta \\ -b\sigma_{\phi\phi} \\ 0 \end{pmatrix} dz \tag{15}$$

Substituting for the expressions of the stresses inside and outside the inclusion and integrating we obtain the total force on the segment. To obtain the force on the node 2 we weight the expression above with the first order function $\frac{z-h}{L}$ and then the integration is perform.

For the forces outside the precipitate we have a total force on the dislocation segment from integrating

$$\overrightarrow{f}^2 = \int_{z_1}^{z_2} \overrightarrow{df}^T \tag{16}$$

given as

$$\overrightarrow{f}^T \overrightarrow{i} = \frac{ER_i^2 c}{H_j^2 \left(H_j^2 + z^2\right)^{\frac{3}{2}} (\nu + 1)} \left(H_j^3 b_3 - b_2 z \left(3H_j^2 + 2z^2\right) + b_2 \left(H_j^2 + z^2\right)|z|\right)\Big|_{z_1}^{z_2} \tag{17}$$

$$\overrightarrow{f}^{T}\overrightarrow{j} = -\frac{ER_i^2 b_1 c\,|z|}{H_j^2\sqrt{H_j^2+z^2}\,(\nu+1)}\Bigg|_{z_1}^{z_2} \tag{18}$$

The force on node 2 is given as

$$\overrightarrow{f}^{2} = -\left(\frac{h}{L}\right)\overrightarrow{f}^{T} + \int_{z_1}^{z_2}\frac{z}{L}d\overrightarrow{f}^{T} \tag{19}$$

Resulting in

$$\overrightarrow{f}^{2}\overrightarrow{i} = -\left(\frac{h}{L}\right)\overrightarrow{f}^{T}\overrightarrow{i} - \frac{ER_i^2 c\left(-H_j^3 b_2\,|z| + H_j b_2\left(H_j^2+z^2\right)|z| + b_3 z^4\right)}{H_j L_j\left(H_j^2+z^2\right)^{\frac{3}{2}}(\nu+1)\,|z|}\Bigg|_{z_1}^{z_2} \tag{20}$$

and

$$\overrightarrow{f}^{T}\overrightarrow{j} = -\left(\frac{h}{L}\right)\overrightarrow{f}^{T}\overrightarrow{j} + \frac{ER_i^2 b_1 c}{L_j\sqrt{H_j^2+z^2}\,(\nu+1)}\Bigg|_{z_1}^{z_2} \tag{21}$$

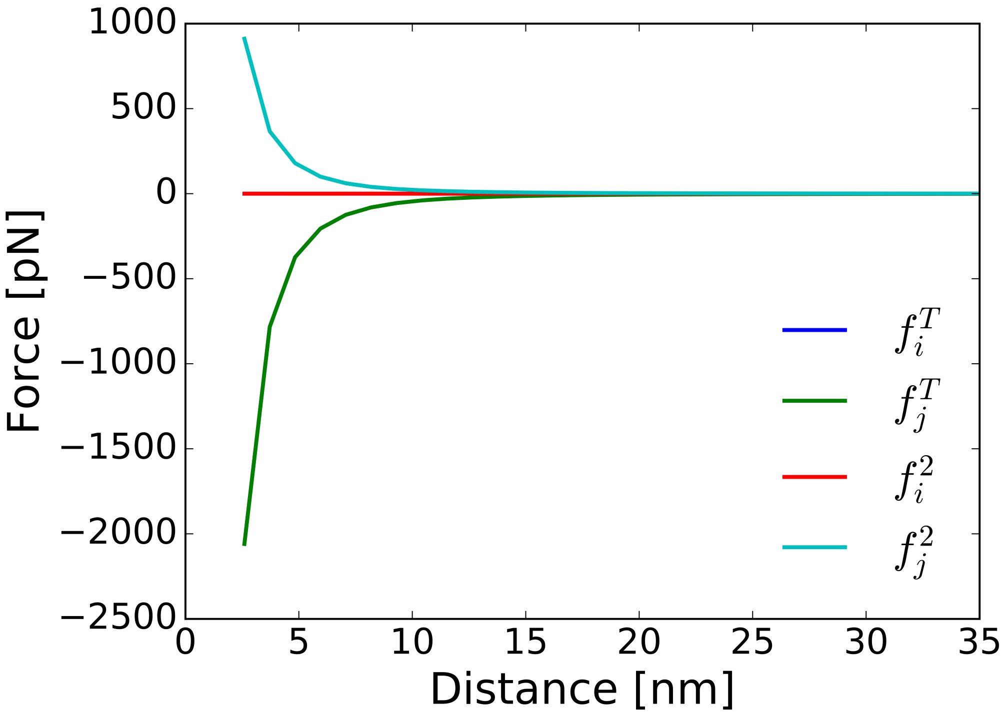

Figure S5: Forces (total and on node 2) on a pure edge dislocation segment outside a spherical inclusion with increasing distance H to the center of the inclusion. i and j is given in figure 1. And the segment is oriented along k, glideplane normal along j and with burgers vector along i. The segment goes from $k = 0$ to $k = 2$

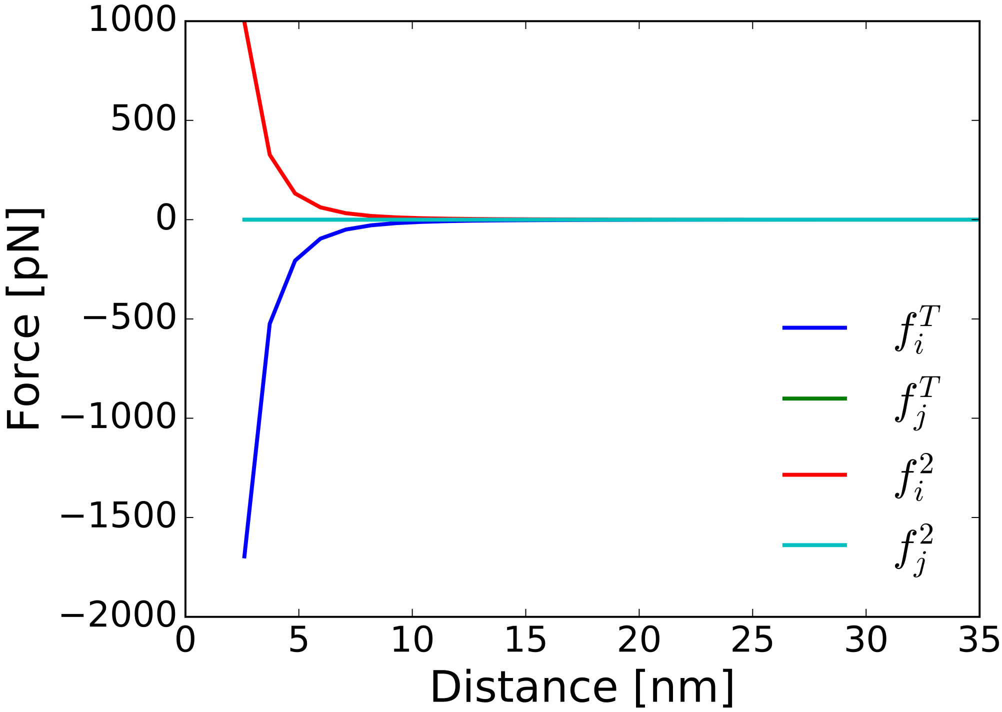

Figure S6: Forces (total and on node 2) on a pure screw dislocation segment outside a spherical inclusion with increasing distance H to the center of the inclusion. i and j is given in figure 1. And the segment is oriented along k, glideplane normal along j and therefore also with burgers vector along j. The segment goes from $k = 0$ to $k = 2$