Supporting Online Material for

The Chemistry of Deformation: How Solutes Soften Pure Metals
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The Chemistry of Deformation: How Solutes Soften Pure Metals

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Supporting material: details of methods and model parameter values.

Direct solute-dislocation interaction.

We calculate total energies and forces for the dislocation and dislocation-solute systems using carefully converged ab initio calculations, performed with vasp (S1, S2). VASP is a plane-wave based code using ultra-soft Vanderbilt-type pseudopotentials (S3) as developed by Kresse and Hafner (S4). The calculations were performed using the local-density approximation as parameterized by Perdew and Zunger (S5). The Mo pseudopotential uses a Kr core atomic reference configuration with 5s- and 4d-electrons as valence; the 5d solute pseudopotentials use a Xe core atomic reference configuration with 6s- and 5d-electrons as valence. A plane-wave kinetic-energy cutoff of 230 eV with a $1 \times 1 \times 4$ k-point mesh and a Methfessel-Paxton smearing of 0.1 eV is sufficient to converge the large dislocation supercells. With these parameters, the lattice constant of Mo is $a_0 = 3.0996\AA$, and the elastic constants are $C_{11} = 504$ GPa, $C_{12} = 179$ GPa, and $C_{44} = 92$ GPa. The bulk shear modulus connected with motion of $\frac{1}{2}[111]$ dislocations is $\mu = 135$ GPa. For all geometries, we relax atomic positions until the forces are less than 5 meV/Å.
The single $\frac{1}{2}[111]$ screw-character dislocation is placed in a periodic cell and relaxed using the Green function boundary condition (GFBC) method. A periodic cell of $5[11\bar{2}] \times 9[\bar{1}10] \times [111]$ (a rectangular slab of $38\text{Å} \times 39.5\text{Å} \times 5.37\text{Å}$) contains 540 atoms with a periodic repeat length of two Burgers vectors in the dislocation line direction. The initial geometry for the pure Mo dislocation is the displacement field from anisotropic elasticity theory, which is relaxed using GFBC. The atoms in the cell are separated into three regions based on their planar distance from the dislocation core: region I contains 122 atoms less than 10.5Å from the core, region II are the 156 atoms between 10.5Å and 15.6Å, and region III are the remaining 262 atoms. This gives a buffer region of 7Å between periodic images of region II atoms. The GFBC method is an iterative method using atomistic forces combined with the long-range elastic response of the material through the lattice Green function (LGF). First, the atoms in region I are fully relaxed using ab initio forces while holding atoms in regions II and III fixed, producing an increase of forces in region II and III. Then, the LGF is used to displace atoms in all three regions using the ab initio forces on atoms in region II:

$$\vec{u}(\vec{R}) = \sum_{\vec{R}'} G(\vec{R} - \vec{R}') \vec{f}(\vec{R}')$$

where $\vec{R}'$ only varies over atoms in region II and $G(\vec{R} - \vec{R}')$ is the (tensor) LGF. This displaces all atoms as if they were part of an infinite bulk rather than a periodic cell. The relaxation cycle is continued between full relaxation of region I and LGF relaxation of region II until forces in both regions I and II are reduced below 5 meV/Å. The final geometry represents the core geometry of a single isolated screw-character dislocation.

The screw-character dislocation core maintains the eight nearest-neighbor coordination found in bulk. In bcc Mo, each atom has eight neighbors at 2.73Å, where we identify neighbors at distances less than 3Å. We find atoms in the dislocation core have eight neighbors: two atoms at a distance of 2.65Å, two at 2.73Å, and four at 2.80Å. However, the dislocation core produces
a different bonding environment than the bulk due to substantial bond-bending. We expect that solutes will respond to differently in these two environments.

Once the pure Mo dislocation is relaxed, individual symmetry-distinct Mo atoms in the dislocation core are replaced with single solute atoms and relaxed. Since the interaction energy is only defined at lattice sites, and bicubic spline is used to smoothly interpolate energy values. The difference in (relaxed) energy as the solute is placed further from the dislocation core defines the interaction energy. Only atoms in region I are relaxed. For the solute calculations, LGF relaxation is not performed so that the contributions to the the total energy of different configurations from the atoms in region II and III do not change for each solute position. We follow this procedure to avoid any ambiguity in the contribution from the long range elastic field to the total energy. By not relaxing region II, an rms force buildup of 30 meV/Å was seen for the solute positions furthest from the dislocation center (and hence, closest to the boundary for region II). Using the LGF value of \( G(\vec{R} - \vec{R}') = 0) = 0.05\,\text{Å}^2/\text{eV} \) with the \( f_{\text{rms}} \), the energy error can be estimated as \( N_{\Pi} u_{\text{rms}} f_{\text{rms}} \); the rms displacement \( u_{\text{rms}} \) is \( \sim 1.5\text{mÅ} \). Thus, the estimated energy error is 7 meV, far less than the smallest calculated interaction energy of 100 meV.

The effect of the periodic repeat length on the solute-dislocation interaction energy appears to be small compared to the interaction energy itself. A single calculation with Re in the core of a dislocation with repeat length of 4 Burgers vectors (but smaller in-plane dimensions of \( 4[11\bar{2}] \times 7[\bar{1}10] \)) showed similar changes in the core geometry compared with a 2 Burgers vectors repeat length. Hence, the shorter repeat length seems reasonable for computing the interaction energy. Moreover, as the interaction energy is the difference between the energy of the solute in the core and the energy of the solute at a further site in the dislocation, the effect of the solute-solute interaction on the solute-dislocation energy is approximately removed by taking this energy difference.

To calculate the bulk-based misfits (shear modulus, size, and atomic-row misfits), bulk su-
percells were used with corresponding k-point meshes. Size and shear modulus misfits were calculated in 16 atom $2 \times 2 \times 2$ simple cubic cells with a single solute, corresponding to a concentration of 6.25%, and a $11 \times 11 \times 11$ k-point mesh. Several volumes were calculated, and the atomic positions relaxed in each. The pressure for each volume was fit to a quadratic to extract the new equilibrium volume and bulk modulus. At the new equilibrium volume, a series of volume-conserving strains corresponding to $e_{xy}$ and $e_{xx} - e_{yy}$ were calculated, again relaxing atom positions in the unit cell. The stress tensor versus strain gives the new $C_{44}$ and $C_{11} - C_{12}$ for the Mo-solute lattice. Assuming linear variation with concentration, both $a_0^{-1} da_0/dc (c = 0)$ and $\mu^{-1} d\mu/dc (c = 0)$ were calculated. The atomic-row misfit calculation used a 192 atom supercell $3[11\bar{2}] \times 4[\bar{1}10] \times 2[111]$, which has a repeat length of 4 along the Burgers vector, with a $2 \times 2 \times 2$ k-point mesh. A single atom in one row is replaced with solute, and the entire row displaced along [111]; the energy versus displacement is compared for the pure Mo case with the single solute case. The stiffness misfit is extracted using a concentration of 25%.

For the Peierls misfit, a single solute atom is placed in an atomic row in the core of dislocation (c.f. Fig. 2) with periodic repeat distance of two Burgers vectors. The periodic boundary conditions correspond to a repetition along the dislocation line of solute-bulk. The dislocation is relaxed, and then used as the reference configuration for displacement. The two atoms in the core (one solute, one Mo) are displaced in the [111] direction, and the total energy computed. The relaxed initial energy is subtracted to give the change in energy from displacement only. To eliminate the contribution from the Mo atom along the line, the displacement energy for a pure Mo dislocation using a periodic repeat distance of one Burgers vector is subtracted. Summarizing, this gives $\delta E(\text{solute, displ.})$ as

$$\delta E(\text{solute, displ.}) = [E_{2 \text{row}}(\text{solute + Mo, displ.}) - E_{2 \text{row}}(\text{solute + Mo, relaxed})]$$

$$- [E_{1 \text{row}}(\text{Mo, displ.}) - E_{1 \text{row}}(\text{Mo, relaxed})],$$

which is the change in energy per solute atom as a function of displacement along the dislocation.
row. Hence, $\delta E$ approaches zero quadratically for all solutes. The effect of periodic repeat-length on the row energy change is expected to be similarly small as the effect on interaction energies.

Table S1 illustrates how traditional models have attempted to approximate the change in the Peierls stress by referencing changes to bulk crystalline environments, compared to the direct calculation of the change in the dislocation core. Changes in the Peierls stress with solute concentration $c$ can be measured as a zero-concentration misfit parameter $\tau^{-1}d\tau/dc(c = 0)$. The misfit modifies stress scales in the solid-solution model using a linear approximation: $\tau(c) = \tau(0)(1 + c\tau')$, where $\tau'$ is the direct misfit from Table S1. The three approximations to the misfit $\tau'$ come from changes in (1) the bulk shear modulus $\mu$, (2) the effective stacking fault energy, and (3) the stiffness for an atomic row in bulk Mo displaced along $\frac{1}{2}[111]$. The approximations assume that the Peierls stress should have a similar relative change with solutes as quantities derived in a bulk lattice. The difference between these approximations and the direct misfit illustrate the influence of the dislocation geometry on the bonding environment a solute experiences: All approximations shown in the first three columns of Table S1 are quantitatively wrong, while some (such as the modulus misfit) predict incorrect signs for the Peierls misfit.

Table S2 shows the interaction energy computed using two bulk-based approximations compared to the direct calculation of the dislocation-solute interaction. The interaction energy is the difference between the energy of the solute in the dislocation core and at the furthest site from the dislocation, corresponding to a distance of $2.37b$. The trend is for lower $d$-electron solutes (Hf, Ta) to have a repulsive interaction, and higher $d$-electron solutes (Re, Os, Ir, Pt) to have increasingly attractive interactions. The interaction energy is traditionally approximated using the modulus misfit ($S7$). We have also used changes to the bulk atomic row energy used in the dislocation geometry. Such approximations are quantitatively incorrect (by as much as a factor
of 2), and can give an incorrect sign for the interaction. These differences show these are not purely mechanical effects, as implied by traditional models, and that it is necessary to correctly treat chemistry and dislocation geometry.

**Solid-solution model.**

Our solid-solution model uses thermally activated motion of dislocations by double-kink nucleation and kink migration (see e.g. prior models \((S8, S7, S9, S10)\)). Applied stress decreases the enthalpy barriers to nucleate a double-kink or migrate kinks, and solutes change the maximum value and the stress dependence of these barriers. The functional forms for the enthalpy barriers come from elasticity theory, and the parameters for pure Mo come from experimental results. Previous models, such as Suzuki \((S7)\) and Petukhov \((S9)\), were constrained to use what data was available. We combine elements of \((S7)\) and \((S9)\), recasting them to use the new direct interaction data with modern parameterizations from \((S11)\) and \((S10)\).

Our prediction of yield stress for a given solute concentration and temperature relies on numerical solution of the Orowan equation \((S12)\) given expressions for the average kink velocity under thermal activation. In the Orowan equation \(\dot{\varepsilon} = b\rho_m\bar{v}_{\text{disl}}(\sigma)\), the strain rate \(\dot{\varepsilon}\) is specified by the experiment, the Burgers vector \(b = \sqrt{3/4} \ a_0\) is given by geometry, and the mobile dislocation density \(\rho_m\) is assumed to be approximately equal to the total dislocation density \((10^8 \ \text{cm}^{-2})\). A kink moves along the \((\bar{1}10)\) plane, translating the dislocation by \(\sqrt{2/3} \ a_0\), which is \(0.94b\), thus \(\bar{v}_{\text{disl}}(\sigma) = 0.94b/\bar{t}_{\text{move}}(\sigma)\). The average time to move the dislocation \(\bar{t}_{\text{move}}(\sigma)\) is the sum of the average time to nucleate a stable double-kink and the time to migrate the kinks along the dislocation length. The double-kink nucleation and kink migration rates for a given stress can be computed using specified temperature and solute concentrations with the solute interaction parameters. A bisection bracketing method is used to numerically find the stress
which satisfies the Orowan equation

\[ \dot{\varepsilon} = 0.94 b^2 \rho_m \left( \text{(nucleation rate)}^{-1} + \text{(migration rate)}^{-1} \right)^{-1}. \]

Our double-kink nucleation model in pure Mo (no solutes) follows the form developed by Argon (S10) from elasticity theory, using exponents from Tang (S11), and pure Mo values fit to Davidson’s flow stress data (S13). Both Argon and Tang use the functional form of Kocks et al. (S14). However, Tang fit the exponents to experimental measurements of bcc Ta yield stress, giving

\[ \Delta H_{dk}(\sigma) = \Delta H^0_{dk} \left[ 1 - \left( \frac{\sigma}{\tau_{dk}} \right)^{0.75} \right]^{1.17}. \]

It is assumed that the natural (no solute) barrier for kink-migration is zero, which is consistent with experimental TEM measurements of Mo showing long straight screw-character dislocations. Assuming the kink-migration rate is much faster than the nucleation rate at the yield stress for pure Mo, the enthalpy barrier at zero stress \( \Delta H^0_{dk} \), zero temperature yield stress \( \tau_{dk} \), and attempt frequency \( \nu_{dk} \) can be determined by fitting experimental data for yield-stress at different temperatures using the Orowan equation. Argon parameterizes both \( \Delta H^0_{dk} \) and \( \tau_{dk} \) in terms of a single parameter \( \alpha \) using elasticity theory (S10):

\[ \tau_{dk} = \pi 0.94^{-1} \mu \alpha \quad \text{and} \quad \Delta H^0_{dk} = \frac{\pi^{3/2}}{4} 0.94(\mu b^3)\alpha^{1/2}. \]

The Orowan equation using only double-kink nucleation,

\[ \dot{\varepsilon} = 0.94 b^2 \rho_m \nu_{dk} \exp \left\{ -\frac{\Delta H^0_{dk}}{k_B T} \left[ 1 - \left( \frac{\sigma}{\tau_{dk}} \right)^{0.75} \right]^{1.17} \right\}, \]

simplifies to a non-linear equation for the yield-stress with temperature,

\[ \sigma(T) = \tau_{dk} \left[ 1 - \left( \frac{T}{T_{dk}} \right)^{1/0.75} \right]^{1/1.17}, \]

where \( T_{dk} \) is

\[ k_B T_{dk} = \Delta H^0_{dk} \left[ \ln \nu_{dk} - \ln \left( \frac{\dot{\varepsilon}}{0.94 b^2 \rho_m} \right) \right]^{-1}. \]
Davidson’s flow stress data ($S13$) is fit to this function, and the efficacy of the fit is shown in Figure S1. Given $\tau_{dk} = 3.74 \times 10^{-3} \mu$ ($\mu = 135$ GPa is the shear modulus) and $T_{dk} = 544$K, we find $\alpha = 1.1235 \times 10^{-3}$ and $\nu_{dk} = 2.3 \times 10^{10}$ s$^{-1}$, which gives $\Delta H_{dk}^0 = 0.78$ eV.

To model solute effects on double-kink nucleation requires two elements: (1) the change in stress scales due to the introduction of solutes, and (2) the changing environment of nucleation centers containing a solute. The former piece is treated by Argon ($S10$) by changing $\alpha$ with the shear modulus misfit. We do this in our model by scaling $\tau_{dk}(c)$ with solute concentration using the Peierls misfit $(1 + c\tau')$ and scaling $\Delta H_{dk}^0(c)$ using $(1 + c\tau')^{1/2}$. Hence, we retain the scaling of the enthalpy barrier with stress, but instead use the change in the stiffness for moving a dislocation as our misfit. To handle the change in environment of nucleation centers, Petukhov ($S9$) shifted the overall enthalpy barrier by the interaction energy for a fraction of sites $c$. We incorporate this effect by adding $E_{int}$ to $\Delta H_{dk}^0(c)$ for $c$ of the sites, leaving $(1 - c)$ sites with the bare double-kink nucleation barrier. This gives a total nucleation rate of

$$(\text{nucleation rate}) = \nu_{dk} \exp\left\{-\frac{\Delta H_{dk}(\sigma, c)}{k_B T}\right\}\left\{(1 - c) + c \cdot \exp\left\{-\frac{E_{int}(\sigma)}{k_B T}\right\}\right\}.$$  

The stress dependence of $E_{int}(\sigma)$ is the same stress dependence as $\Delta H_{dk}$:

$$E_{int}(\sigma) = E_{int}\left[1 - \left(\frac{\sigma}{\tau_{dk}(c)}\right)^{0.75}\right]^{1.17}.$$  

Our kink-migration model follows Suzuki’s formulation ($S7$), as parameterized by Argon ($S10$). In Suzuki’s model, the rate-limiting step of kink-migration is the time to overcome the largest cluster of solutes to occur along the length of dislocation between two superjogs. The superjogs are pinning sites of the dislocation which are unable to move. We assume that this pinning is due to forest dislocations, and hence the distance between pinning sites $\Lambda \sim \rho^{-1/2}$, where $\rho$ is the dislocation density. For our case, $\Lambda \sim 10^4 \text{Å}$, however we will show below that changes in $\Lambda$ by an order of magnitude produce only modest changes in the model.
The largest cluster of solutes is determined statistically from the average number of solutes that will appear in a kink \((S7, S10)\). By elasticity theory, a kink has a “width” (distance along the dislocation line from start to finish) of \(w_k = b^2/0.94\alpha^{-1/2}\), where \(\alpha\) is the parameter from the double-kink nucleation model, and for Mo, \(w_k = 14b\). There are three atoms in the center of a dislocation per Burgers vector, so on average there are \(n = 3(w_k/b)\) solutes per kink. Assuming there is no interaction between the solutes, the probability of finding a cluster of \(m\) solutes in a kink given the average number of solutes per kink \(n\) is the Poisson distribution

\[
P(m, n) = 1 - \frac{1}{2\pi} \int_m^\infty \exp\left(-\frac{m^2}{4n}\right) \, dm.
\]

For \(m > 4\sqrt{2n}\),

\[
P(m, n) \approx \frac{1}{4\pi} \frac{\exp\left(-\frac{m^2}{4n}\right)}{\sqrt{m^2/4n}}.
\]

The largest cluster size, \(m_0\), is the cluster with probability of 1 of being found in the \(\Lambda/w_k\) segments along the dislocation line between superjogs: \(P(m_0, n)(\Lambda/w_k) = 1\). The closed-form expression for \(m_0\) is

\[
m_0 = \sqrt{\frac{3}{\pi}} \left(\frac{\Lambda}{\sqrt{w_k}b}\right) \exp\left[-\frac{1}{2} W\left(\frac{(\Lambda/w_k)^2}{2\pi}\right)\right] \sqrt{c},
\]

where \(W\) is the Lambert W-function.\(^1\) Evaluating the geometric terms gives \(m_0 = 25\sqrt{c}\). This geometric prefactor depends on \(\Lambda\) (and, hence, \(\rho\)), but only weakly. Figure S2 shows the change in the prefactor while \(\rho\) varies across four orders of magnitude (two order of magnitude in \(\Lambda\)); it has a maximum of 31 and minimum of 17. Hence, the model is fairly insensitive to the exact value of \(\Lambda\), provided it falls in a physically reasonable range.

Given the largest solute cluster \(m_0\), the kink-migration rate is given by the enthalpy barrier to overcome this cluster. The cluster is assumed to have a total interaction energy of \(m_0|E_{\text{int}}|\) with the dislocation. Argon \((S10)\) writes the kink-migration enthalpy barrier using a Kocks \textit{et al.}\(^1\)

\(^1\)The Lambert W-function is the inverse function of \(f(W) = We^W\).
form

$$\Delta H_{\text{km}}(\sigma, c) = \Delta H_{\text{km}}^0(c) \left(1 - \frac{\sigma - \tau_{\text{athermal}}(c)}{\tau_{\text{km}}(c)}\right)^{3/2},$$

where the exponents are a “best fit” using a Peierls-Nabarro model for the dislocation motion with a Gaussian interaction energy profile. The stress-free energy barrier $\Delta H_{\text{dk}}^0(c) = m_0|E_{\text{int}}|$. The kink-migration stress $\tau_{\text{km}}$ (also based on the Peierls-Nabarro model with Gaussian interaction) is

$$\tau_{\text{km}}(c) = \frac{2}{3} \mu (1 + c \tau') m_0 |E_{\text{int}}| \left(\frac{b}{w_k}\right)^{0.94^{-1}}.$$

The athermal, or “plateau” stress becomes the limiting stress at high temperatures. This accounts for the experimental fact that above $\sim 15\%$ of the melting temperature, bcc have yield stresses that are roughly temperature-independent. The bare athermal stress for pure Mo comes from Davidson’s data (S13): $\sim 3.6 \times 10^{-4}\mu$. Solutes increase this athermal stress, akin to traditional solid-solution hardening,

$$\tau_{\text{athermal}}(c) = \mu (1 + c \tau') \left[3.6 \times 10^{-4} + \frac{b F_{\text{max}}}{\mu b^3} c\right],$$

where $F_{\text{max}}$ is the maximum interaction force a solute produces on a dislocation. For all of the solutes we studied, $F_{\text{max}} \approx E_{\text{int}}/3\bar{A}$. The final kink-migration rate is

$$\text{(migration rate)} = \nu_D \exp \left(-\frac{\Delta H_{\text{km}}(\sigma, c)}{k_B T}\right),$$

where the attempt frequency is the Debye frequency $\nu_D = 5 \times 10^{11}\text{s}^{-1}$.

Finally, the range of the solute-dislocation interaction must be accounted for in the solid-solution model. In the elasticity models, and hence our solid-solution model, the interaction of the solute with the dislocation is assumed to be short-ranged. That is, once the dislocation translates by one lattice site, it no longer feels the effect of the solute. However, the actual solute interaction is extended over several lattice sites. To make the solute interaction calculated atomistically compatible with the interaction energy used in the solid solution model requires
that $E_{\text{int}}$ be the change in interaction energy from one lattice site to an adjacent one along the $(\bar{1}10)$ plane. For all of the $5d$ solutes computed, this was found to be one-half of the full $E_{\text{int}}$ found in Table 2 of the paper. This factor must be used to scale the interaction energy from the ab initio results for use in the solid-solution model. However, this change must be evaluated on a case-by-case basis for other systems and other solutes as it reflects the range of chemical interactions near and around the dislocation core.

**Softening with concentration and temperature.**

While there are hardness measurements for the $5d$ solutes Hf through Pt in Mo from Stephens and Witzke (S15), the only known single crystal flow-stress data for Mo with $5d$ solutes is Davidson’s work on Mo-Re (S13). Predicting hardness is theoretically difficult, as it represents the response of a metal to indentation (which creates strain gradients) rather than uniform stress. The lack of yield- or flow-stress data for all of the alloys investigated requires us to predict hardness using a linear correlation between the Vickers hardness number (VHN) and the flow-stress from our model. The correlation was found using a linear fit of the VHN for pure Mo at four temperatures against the flow stress predicted from our earlier fit to Davidson’s data. This allowed us to interpolate Davidson’s data to the temperatures used in the hardness measurements. Figure S3 shows two attempts at a linear fit; the simple scaling relation between VHN and flow-stress, while perhaps more physically intuitive, deviates from the experimental data in a non-systematic manner. To avoid the additional error introduced by correlation when comparing our predictions to the experiments, we chose to use the linear relation which has smaller deviations: $\text{VHN} = 45 + 1.2 \times 10^5 (\text{FS}/\mu)$

**References and Notes**

Figure S1: Parameterized fit of Davidson’s flow stress at 10% strain for pure Mo (S13) at 77, 150, 250, 300, 350, and 425K. This fit determines the double-kink attempt rates, zero-stress enthalpy, and zero-temperature critical stress.
Figure S2: Dependence of the geometric prefactor for $m_0 \propto \sqrt{c}$ in Suzuki’s model with the dislocation density. The dislocation forest density provides pinning sites separated by $\Lambda = \rho^{-1/2}$. This distance determines the statistical average largest solute cluster that a kink must overcome to move the dislocation forward. Even as $\rho$ varies over four order of magnitude, the prefactor only varies from 17 to 31.
Figure S3: Linear correlation between predicted flow stress for pure Mo fit from (S13) and hardness measurements (Vickers hardness number) for pure Mo from (S15). The direct scaling relation is not an ideal fit; in order to reduce the error induced from correlating hardness to flow stress, we use the linear relation which has smaller error.
Table S1: Approximations for the change in the Peierls stress compared to the direct calculation of the change in the core restoration force (from Fig. 2). All changes are reported as “misfits”: relative change $\tau^{-1}d\tau/dc(c = 0)$. The simplest approximation, labeled “Modulus,” is the change in the bulk shear modulus connected with motion of $\frac{1}{2}$[111] screw-character dislocations. The next approximation, labeled “GSF,” is the change in generalized stacking fault energy, a useful approximation for edge dislocations (values from (S16) at 8 at.% concentration). A better approximation, labeled “Row,” is the change in the stiffness to move an atomic row with a solute in bulk Mo. The change in the Peierls stress, labeled “Direct,” is the change in resistance to moving an atomic row in the core of the screw-character dislocation when a solute is introduced.

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Table S2: Dislocation-solute interaction energy in eV approximated using the modulus misfit (S7), the change in the bulk atomic row energies, and calculated directly. Both the approximate calculations deviate from the true interaction, though the atomic row misfit calculation captures the trend of repulsive interactions for solutes with lower $d$-electron concentrations (Hf, Ta) and attractive interactions with higher $d$-electron solutes (Re, Os, Ir, Pt).

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