Supporting Information for
Plastic Forming of Metals at the Nanoscale: Interdiffusion-Induced
Bending of Bimetallic Nanowhiskers

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Additional results:

Estimating the bending of the NW#1 at 25°C due to lattice mismatch strain and island-zipping stress

We consider two physical reasons for the observed bending in the as-synthesized NW#1 at 25 °C, i.e. the lattice mismatch strain at the coherent single-crystalline (SX) Fe-Au interface, and the strain induced by the closing the nano-cavities at the grain boundaries (GBs) in the poly-crystalline (PX) Fe layer.

Let us first estimate the contribution from the lattice mismatch strain. Because there is no coherency strain in the PX Fe layer adjacent to the incoherent PX Fe-Au interface, we will only consider the lattice mismatch strain at the coherent SX Fe-Au interface. Here, we use a simplified model, see Figure. S2, in which the Au NW has a square cross-section with four {100} facets, with the SX Fe layer covering one facet in the Bain orientation relationship with the Au NW. The mismatch strain between (011)_{Au}//(010)_{Fe} on the Au NW can be estimated as \( \varepsilon_{m} = \frac{d_{Fe(010)} - d_{Au(011)}}{d_{Au(011)}} = -0.0059 \), where \( d_{Fe(010)} = 0.2867 \) nm and \( d_{Au(011)} = 0.2884 \) nm are the interplanar spacings in Fe and Au, respectively.

To estimate the radius of curvature, \( R \), the Timoshenko formula\(^1\) describing the bending of bimetallic beams is employed here:

\[
R = \frac{E_{Fe} h_{Fe}^4 + 4 E_{Fe} E_{Au} h_{Fe}^2 h_{Au} + 6 E_{Fe} E_{Au} h_{Fe}^2 h_{Au}^2 + 4 E_{Fe} E_{Au} h_{Fe} h_{Au}^3 + E_{Au}^2 h_{Au}^4}{6 E_{Fe} E_{Au} (h_{Fe} + h_{Au}) h_{Fe} h_{Au} \cdot \varepsilon_{m}} \tag{S1}
\]

where \( E_{Fe} = 125 \) GPa and \( E_{Au} = 82 \) GPa are the Young’s moduli of Fe and Au along [001] and [011] crystallographic directions, respectively. \( h_{Fe} = 160 \) nm and \( h_{Au} = 200 \) nm are the thicknesses of the Fe and Au constituents, respectively, estimated from Figure S2 (d).

The radius of curvature, \( R \), is estimated to be 40 µm, which is somewhat larger than the measured one, 23±1 µm, in Figure 1. This difference could be caused by the tensile stress developed in the PX Fe layer during growth, and compressive strain in the Au NW in the vicinity of the interface, see Figure S3. In particular, the drive of the system to close the long and narrow nano-cavities at the GBs induces the tensile stress in the film, similar to the island zipping stress during the Volmer–Weber film growth. Here we estimate the average tensile stress, \( \langle \sigma \rangle \), using Nix-Clemens model:\(^2\)

\[
\langle \sigma \rangle = \left[ \left( \frac{1 + \nu}{1 - \nu} \right) E \cdot \left( \frac{2 \gamma_s - \gamma_{gb}}{r} \right) \right]^{\frac{1}{2}} \tag{S2}
\]

where \( v, E, \gamma_s, \) and \( \gamma_{gb} \) are the Poisson’s ratio, the Young’s modulus, the surface energy and the grain boundary energy of ferrite \( \alpha \)-Fe, which were chosen to be 0.3, 210 GPa, 2.1 J/m\(^2\) and 1 J/m\(^2\), respectively.\(^3\) The parameter \( r \) denotes the radius of the grain and its chosen value is 33 nm, based on the measurements in Figure S2(e). The average tensile stress, \( \langle \sigma \rangle \), is estimated to be 19.1 GPa. Though this high stress may partially relax by various plasticity and diffusion mechanisms, our results indicate that the residual internal stress in the PX Fe layer is tensile, and contributes to the bending of the as-prepared NW.
Estimating the bending of the NW#1 at 300 °C due to the mismatch of thermal expansion coefficients

The radius of curvature of NW#1 changed from $23\pm 1 \, \mu m$ to $18\pm 1 \, \mu m$ upon heating to 300 °C, which indicates an increase of the tensile stress in Fe coating. We attributed this phenomenon to the mismatch in the coefficients of thermal expansion of Au ($14.2 \cdot 10^{-6} \, ^{\circ}C^{-1}$) and Fe ($11.4 \cdot 10^{-6} \, ^{\circ}C^{-1}$). This mismatch resulted in a thermal strain of $-0.0008$ upon heating the NW#1 from room temperature (25 °C) to 300 °C. This thermal strain has to be added to the lattice mismatch strain of $-0.0059$, resulting in a total mismatch strain of $-0.0067$. According to Eq. (S1) this increase of strain results in the decrease of the NW radius of curvature from 40 μm to 36 μm, in qualitative agreement with the experimental data.

Kinetics of the nano-cavities healing in the PX Fe layer at 300 °C

We observed that while the radius of curvature of the NW#1 decreased to $R = 18\pm 1 \, \mu m$ upon heating to 300 °C, it has not fully recovered to its original value $R = 23\pm 1 \, \mu m$ after the NW has been cooled down to 25 °C. A slight decrease of the radius of curvature upon the full heating-cooling cycle (from 23±1 to 21±1 μm) is related with the irreversible processes occurring in the NW at elevated temperatures. We attribute this phenomenon to the healing of nano-cavities in the Fe layer, which results in a volume shrinkage of the Fe constituent and concomitant increase of the tensile stress in the layer. The healing and annihilation of the nano-cavities at elevated temperatures was demonstrated in the ex-situ heat treatment, see Figures S4 and S5. We assume that the healing process occurred via Fe atoms diffusion through a GB connected to the nano-cavity. The GB itself plays a role of a source of Fe atoms (or a sink of vacancies), which in turn contributes to the increase of tensile stress in the Fe coating. To prove this hypothesis, we propose a model to estimate the time required for Fe GB diffusion to heal a slit-shaped nano-cavity. In our model, the main driving force for the nano-cavity healing is the decrease of energy associated with replacing two free Fe surfaces (side surfaces of the slit) with an Fe GB.

Let us consider a slit-shaped nano-cavity with the thickness $h=3 \, nm$ and total length $L_0= 50 \, nm$, located at the distance $l_0 = 20 \, nm$ away from the Fe-Au interface (Figure S6). A GB in the PX Fe layer is connected to the tip of the nano-cavity. The depletion of Fe atoms at the GB and their diffusion towards the nano-cavity lead to the latter retraction and increase of the distance between the nano-cavity tip and the Fe-Au interface, $l$. We will assume that the Fe grains on both sides of the GB homogeneously drift towards the GB (this way, the generation of additional elastic stresses at the GB associated with normal displacement variations is avoided). In this case, the distribution of chemical potential of Fe atoms along the GB, $\mu(x)$, is a parabolic (second-order) function of the distance, $x$, from the Fe-Au interface, $\mu(x)=ax^2+bx+c$. Additionally, we assume that there is no Fe diffusion flux entering the GB at the Fe-Au interface, $\frac{\partial \mu}{\partial x} \big|_{x=0} = 0$. This boundary condition results in $b = 0$ and $\mu(x)=ax^2+c$.

The chemical potential of Fe atoms averaged over the whole GB length, $l$, is

$$
\bar{\mu}_0 = \frac{1}{l} \int_0^l (ax^2+c) \, dx = \frac{1}{l} \left( \frac{al^3}{3} + cl \right) \quad (S3)
$$
On the other hand, the average chemical potential of Fe atoms that is \( l \) away from the Fe-Au interface can be estimated by adding an infinitesimally thin layer of Fe at the GB, calculating the change of the total energy of the system, and normalizing it by the number of added atoms:

\[
\mu_0 = \frac{\Omega \gamma_s + \gamma_i - \gamma_{Au}}{l}
\]  

(S4)

where \( \Omega \) denotes the atomic volume of Fe; \( \gamma_s, \gamma_i \), and \( \gamma_{Au} \) are the surface energy of Fe, Fe/Au interface energy and surface energy of Au, respectively.

Substituting Eq. (S3) in Eq. (S4) yields

\[
\frac{a l^2}{3} + c = \frac{\Omega \gamma_s + \gamma_i - \gamma_{Au}}{l}
\]  

(S5)

Furthermore, the chemical potential of the Fe atoms on the inner surface of the nano-cavity tip (i.e. at the distance \( l \) from the Fe-Au interface) is

\[
\mu_f = a l^2 + c \approx \frac{\Omega \gamma_{gb} - 2 \gamma_i}{h}
\]  

(S6)

where \( \gamma_{gb} \) is the GB energy of ferrite \( \alpha \)-Fe. The last term on the right hand side of Eq. (S6) is associated with the curvature of the inner surface of the nano-cavity at the tip. Solving Eqs (S5-S6) yields

\[
a = \frac{3 \Omega}{2 l^2} \left( \frac{\gamma_{gb} - 2 \gamma_i}{h} - \frac{\gamma_s + \gamma_i - \gamma_{Au}}{l} \right)
\]  

(S7)

\[
c = \frac{\Omega}{2} \left( \frac{3 \gamma_s + \gamma_i - \gamma_{Au}}{l} - \frac{\gamma_{gb} - 2 \gamma_i}{h} \right)
\]  

(S8)

Then the GB diffusion flux of Fe atoms entering the nano-cavity at the intersection line of the GB and the inner surface of the nano-cavity is

\[
J = -\frac{D_{gb} \delta}{kT} \cdot \frac{\partial \mu}{\partial x} \bigg|_{x=l} = -\frac{D_{gb} \delta}{kT} \cdot \frac{3 \Omega}{l} \left( \frac{\gamma_{gb} - 2 \gamma_i}{h} - \frac{\gamma_s + \gamma_i - \gamma_{Au}}{l} \right)
\]  

(S9)

where \( D_{gb} \) and \( \delta \) are the self-diffusion coefficient of Fe along the GB at 300 °C and the GB width, respectively. \( kT \) has its usual thermodynamic meaning. Assuming the constant width of the nano-cavity, this flux cases the nano-cavity retraction according to

\[
\frac{d l}{d t} = h \cdot \frac{d l}{d t} 
\]  

(S10)

Substituting Eq. (S10) in Eq. (S9) yields

\[
\frac{d l}{d t} = \frac{3D_{gb} \Omega}{kT l h} \left( \frac{2 \gamma_i - \gamma_{gb}}{h} + \frac{\gamma_s + \gamma_i - \gamma_{Au}}{l} \right)
\]  

(S11)
For $l_0 >> h$ the magnitude of the second term on the RHS of Eq. (S11) is small compared to the first term, and the Eq. (S11) can be approximately re-written as

$$\frac{dl^2}{dt} \approx \frac{6D_{gb}\delta \Omega}{kT h^2}\left(2\gamma_s - \gamma_{gb}\right)$$  \hspace{1cm} (S12)

Solving this differential equation yields the following solution for the annealing time required for nano-cavity retraction by the distance $l-l_0$:

$$l^2 - l_0^2 \approx \frac{6D_{gb}\delta \Omega\left(2\gamma_s - \gamma_{gb}\right) t}{kT h^2}$$  \hspace{1cm} (S13)

where $l, l_0, T, h, \delta, \Omega, \gamma_s$ and $\gamma_{gb}$ are chosen to be 70 nm, 20 nm, 573 K, 3 nm, 0.5 nm, 7.1·10^{-6} m²/mol, 2.1 J/m², and 1 J/m², respectively. $D_{gb}$ was chosen in the range between 1.3·10^{-18} m²/s and 2.8·10^{-16} m²/s.\(^5,^6\) The time of nano-cavity retraction estimated with the aid of Eq. (S13) is then in the range from 17 s to 1 h, depending on the GB diffusivity, in good agreement with our experimental observations. Therefore, the nano-cavities healing at the temperature of 300 °C leading to the increase of tensile stress in the Fe coating is feasible on the time scale of our experiment.

Formation of a tilt GB at the mouth of Au layer penetrating into the gap between PX and SX Fe layers

We will consider a simple model of a rectangular gap between two Fe layers which is filled with Au during high-temperature annealing (Figure S8). We will neglect the changes in the geometry of Au NW upon the gap filling, since the total volume of Au penetrating the gap is negligible in comparison to the volume of the Au NW. Thus, the total energy of all surfaces and interfaces only in the region of the gap will be considered. The initial energy per unit of longitudinal length, $E_{total}^{25^\circ C}$, can be written as

$$E_{total}^{25^\circ C} = L\left(\gamma_{1-Fe}^1 + \gamma_{2-Fe}^2\right) + h\gamma_{S-Au}^1$$  \hspace{1cm} (S14)

where $L$ and $h$ are the length and the width of the gap, respectively. $\gamma_{1-Fe}^1$ and $\gamma_{2-Fe}^2$ are the average surface energy of the PX Fe layer, and the energy of the side surface of the SX Fe layer, respectively. $\gamma_{S-Au}^1$ is the energy of exposed Au surface at the entrance to the gap. Assuming that the gap is filled with Au in homoeptaxial orientation relationship with the underlying Au NW yields the following expression for the energy of the filled gap:

$$E_{total}^{500^\circ C} = L\left(\gamma_{1-Fe}^1 + \gamma_{2-Fe}^2\right) + h\gamma_{S-Au}^1$$  \hspace{1cm} (S15)

where $\gamma_{1-Fe}^1$ and $\gamma_{2-Fe}^2$ are the average energy of the PX Fe-Au interface, and the energy of the SX Fe-(277) Au interface, respectively. Another possibility is for the Au layer penetrating the gap to change its orientation, so that a low-energy SX Fe-(100) Au interface is formed on the right side of the gap. In this case, the total energy of the filled gap will be different from the one given by Eq. (S15):

$$E_{total}^{500^\circ C^*} = L\left(\gamma_{1-Fe}^1 + \gamma_{2-Fe}^2\right) + h\left(\gamma_{S-Au}^1 + \gamma_{GB-Au}^*\right)$$  \hspace{1cm} (S16)
where $\gamma_{GB-Au}$ is the energy of the GB formed at the mouth of the Au layer, and the star superscript denotes the change of surface orientation or interface crystallography. For simplicity, we assumed that the cross-sectional length of the newly formed GB is the same as the gap width $h$. Since the anisotropy of surface energy of cubic metals rarely exceeds 2-3%, we will assume $\gamma^1_{S-Fe} \approx \gamma^2_{S-Fe} \approx \gamma_s \approx 2.1 \text{ J/m}^2$, and $\gamma^1_{S-Au} \approx \gamma^2_{S-Au} \approx \gamma_{Au} \approx 1.4 \text{ J/m}^2$. Because the average energy of the PX Fe-Au interface is determined for many different orientations of the Fe grains, we will assume the equal values of $\gamma^1_{In-Fe}$, $\gamma^2_{In-Fe}$, and of the incoherent interface energy, $\gamma^3_{In-Fe}$. We will estimate the values of these energies by the energy value of high-angle GB in Fe, $\approx 1 \text{ J/m}^2$. The density functional theory-based estimates of the energy of the coherent Fe-Au interface, $\gamma^2_{In-Fe}$, yield the values in the range of 0.36-0.5 J/m$^2$. Finally, the energy of high-angle GB in Au will be estimated as one-third of its surface energy, $\gamma^*_{GB-Au} \approx 0.5 \text{ J/m}^2$. Comparing the Eqs (S14)-(S16) reveals that filling the gap between the two Fe layers by Au is energetically favorable for any values of $L$ and $h$. Moreover, for $h < (1-1.3) \cdot L$, the formation of GB by lattice rotation about [011]$_{Au}$ axis leading to establishing a coherency at the SX Fe-Au interface becomes energetically more favorable than homoepitaxial penetration of Au into the gap. The analysis of Figure 4c, d in the main text and Figure S8 demonstrates that $h$ ($<10 \text{ nm}$) $\ll L$ (50-200 nm) and, therefore, the formation of a GB is energetically favorable.

Estimation of the GB Kirkendall effect induced irreversible bending at the temperatures above 300 °C

The NW#1 bent in the opposite direction at 400 °C and 500 °C, indicating that the stress state of the Fe layer changed from tension to compression. We attribute this lateral expansion of the PX Fe layer to the accretion of Au atoms at the GBs in Fe, as observed in the STEM-EDX micrographs, and is shown schematically in Figure. S10. However, due to the high solubility of Fe in Au the diffusion flux of Au along the GBs in Fe can be accompanied by nearly equal flux of Fe atoms in the opposite direction, either leaving the Fe layer and dissolving in the Au NW, or re-distributing along the Fe-Au interface (chemical GB interdiffusion). Thus, Fe atoms leaving the Fe layer may compensate its lateral expansion due to accretion of Au atoms. We will estimate below whether a simple GB interdiffusion with equal partial GB diffusion coefficients of Au and Fe (i.e. full balance of the GB diffusion fluxes) can account for the observed bending of the NW#1.

The diameters of the Fe and Au atoms are 0.2482 and 0.2884 nm, respectively. With the average grain size in the PX Fe layer of 66 nm, replacing one monolayer of Fe at the GB with a monolayer of Au will cause a lateral strain of $6 \times 10^{-4}$, one order of magnitude lower than the initial mismatch strain. Therefore, the simple GB interdiffusion with equal partial GB diffusion coefficients of Au and Fe cannot account for the NW bending in the opposite direction. Let us now assume that Au diffuses much faster than Fe along the Fe GBs (GB Kirkendall effect). In this case, accretion of Au at the GBs will not be accompanied by any significant outdiffusion of Fe. One full monolayer of Au will cause a strain of 0.004, comparable with the lattice mismatch strain. Accommodating two-three monolayers of Au in the Fe GBs will fully compensate the lattice mismatch strain and lead to the NW bending in the opposite direction, in accordance with our experimental observations. From the measurements in Figure S7b, the width of the Au-rich diffusion/segregation layer at the Fe
GBs after annealing at 400 °C and 500 °C for 20 min is about 2 nm. Thus we conclude that the major part of plastic bending of the bi-metallic Au-Fe NW at high temperatures is caused by the GB Kirkendall effect. It should be noted that the formation of “GB diffusion wedges” of the diffuser during the GB Kirkendall effect has been described by Klinger and Rabkin.10

A schematic representation of the atomic and vacancy fluxes during the GB Kirkendall effect is presented in Figure. S10. For simplicity, we assume that the Fe atoms at the GB are immobile. The GB diffusion of Au atoms into the GB in the PX Fe layer causes an equal in amplitude flux of vacancies in the opposite direction. The divergence of this flux describes the material (Au) accretion at the GB and concomitant lattice drift of both grains away from the GB, assuming that the GB is a perfect source of vacancies. It is this lattice drift which causes a lateral strain of the PX Fe layer. The GB vacancy flux emerges at the triple line where the GB contacts the Fe-Au interface. It is then re-distributed along the Fe-Au interface, which is also a perfect sink of vacancies because of its incoherent nature. The divergence of the interface vacancy diffusion flux causes a concomitant lattice drift of the Au NW in the direction of interface. Thus, an overall picture of the mass balance is as follows: the near-interface Au atoms diffuse into the GBs in the PX Fe layer and cause a lateral expansion of the latter. As a result, the diameter of the Au NW is slightly decreasing, and the NW bends in the direction of Au.
Figure S1. Interfaces in bimetallic Au/Fe NW. (a) HAADF-STEM image of the cross-section of a representative NW; (b, c) the SADP and atomic-resolution HAADF-STEM image showing a single-crystalline Fe layer on a Au (100) facet and a coherent interface between them; (d, e) the SADP and atomic-resolution HAADF-STEM images showing a poly-crystalline Fe layer on a Au (111) facet and an incoherent interface between them. Images were taken along the [0\overline{1}1] Z.A. of Au. Adapted with permission from Ref. [11]. Copyright Elsevier, 2020.

Figure S2. Illustration of the initial NW#1 bending due to lattice mismatch strain and island coalescence stress. (a-d) the lattice mismatch strain induced by the heteroepitaxy at the single-crystalline Fe – Au interface; (a) the model of initial configuration; (b) the bending induced by the lattice mismatch strain; (c) additional elastic bending at 300 °C due to the mismatch in thermal expansion coefficients of Au and Fe; (d) the geometric parameters used for the estimation of the NW radius of curvature; (e) Longitudinal cross-sectional TKD band contrast image of the NW#1 illustrating the geometric parameters used for the estimation of island coalescence stress in PX Fe layer.
Figure S3. A demonstration of Fe-Au interface bending due to island coalescence in the PX Fe layer. (a) HAADF-STEM of the cross-section of the Au/Fe NW; (b, c) LAADF and HAADF-STEM images showing the bending of the PX Fe layer – Au interface due to the island coalescence induced tensile stress in the Fe layer; arrows and dashed lines highlight the bent interface; (d, e) atomic-resolution HAADF-STEM image showing the ledges on the interface and a stacking fault (SF) in the Au NW. The formation of interface ledges and a Shockley partial dislocation indicated the strain was partially relieved by plastic deformation. Images were taken along the [0̅11] Z.A. of Au.

Figure S4. Quasi-in-situ demonstration of nano-cavities healing after annealing. HAADF-STEM images (a, b) showing the cross-section of a bimetallic NW in which some nano-cavities in the Fe layer were highlighted by arrows; (c, d) the same NW after annealing at 330 °C for 60 min in RTA exhibited much fewer nano-cavities. The atomic resolution HAADF-STEM images of (b, d) demonstrate that the Au-Fe interface at the facets intersection migrated towards Fe after annealing. Images were taken along the [0̅11] Z.A. of Au.
Figure S5. Quasi-*in-situ* demonstration of nano-cavities healing and Au penetration into Fe after annealing. HAADF-STEM images (a, b) showing the cross-section of a bimetallic NW in which some nano-cavities in the Fe layer were highlighted by arrows; (c, d) the same NW after annealing at 400 °C for 7 min in RTA exhibited much fewer nano-cavities. The enlarged HAADF-STEM images of (b, d) demonstrate the diffusion and penetration of Au into the nano-cavity at the intersection of Au facets. Images were taken along the [0̅1̅1] Z.A. of Au.

Figure S6. The geometric parameters of the model of a Fe nano-cavity healing by grain boundary (GB) diffusion mechanism. (a, b) HAADF-STEM images showing a representative nano-cavity in the Fe layers; (c) the schematic illustration of the nano-cavity.
Figure S7. Energy minimization approach employed to explain the formation of tilt GB at the “mouth” of Au layer penetrating into the Fe nano-cavity.
Figure S8. Lattice distortion and deformation twinning in bent NW#2 characterized by TKD and LAADF. (a) the CCDF image of the longitudinal cross-section of NW#2; (b) the misorientation map of the Au NW where the reference location is pointed by the white cross. The legend shows the range of misorientations (1°-12°); (c, d) the orientation images showing the twin boundary (TB) and misorientation line profile from the line scan (LS); (e) LAADF image showing the twin boundaries in the cross-section normal to the NW axis [011]Au.

Figure S9. Au atoms accretion at the GBs in Fe causing lateral expansion of the Fe layer and the NW bending towards Au. The HAADF-STEM image-based measurement of the width of Au diffusion/segregation layer at the Fe GB after the in-situ annealing at 500 °C.

Figure S10. Schematic illustration of Au and vacancy diffusion fluxes during the GB Kirkendall effect. For simplicity, we assumed that only Au atoms diffuse along the GBs in Fe. Only one GB in the PX Fe layer is shown. The divergence of the vacancy flux along the GB and along the Fe-Au interface causes the lattice drifts.
Figure S11. The evolution of the cross-sectional dimensions of the NW#3 after annealing at 600 °C for 30 min. The estimation was based on the measurements of the areas in HAADF-STEM images before (a) and after (b) annealing. Images were taken along the [0\overline{1}1] Z.A. of Au.

Figure S12. The formation of an incoherent twin boundary (ITB) induced by interface migration and bulk Fe-Au interdiffusion. (a) an atomic resolution HAADF-STEM image showing an ITB (211) formed in the vicinity of the incoherent Au – PX Fe interface after annealing at 350 °C for 30 min. (b) the lower magnification HAADF-STEM image showing the nano-roughness of the interface which indicates the migration process. Images were taken along the [0\overline{1}1] Z.A. of Au.
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