Reverse plasticity in single crystal silicon nanospheres

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Abstract

Nanoparticles in the range of 20 to 100 nm in size can be deposited, isolated, and individually probed for their mechanical properties. With a hypersonic plasma particle deposition technique, this has been successfully accomplished for silicon and titanium. We have already shown that silicon nanoparticles are superhard in the 30 to 50 GPa range after work hardening (Gerberich, W.W., Mook, W.M., Perrey, C.R., Carter, C.B., Baskes, M.I., Mukherjee, R., Gidwani, A., Heberlein, J., McMurry, P.H., Girshick, S.L., 2003a. Superhard silicon nanospheres. J. Mech. Phys. Solids 51, 979). At the same time when small nanospheres are compressed, a fraction of the plastic strain is reversed after unloading. Initially, the amount of reverse dislocation motion was small but appeared to accelerate once a threshold strain was reached. The cumulative reverse plastic strain from repeated loading of the same nanosphere appeared to increase from less than 0.04 to approximately 0.4 as cumulative strain increased from 0.2 to 0.6. For large strains then, it appears that a greater amount of plastic strain is recovered after unloading. This can at least partially be understood in terms of the enormous

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back stress developed at the small scale when dislocations are only a few nm apart. As the ramifications to nanoscopic features on MEMS, micromachines and magnetic recording devices is considerable, it is desirable to understand if a length scale can be developed for such phenomena. In terms of classic dislocation theory an attempt is made. Problems and prospects are discussed with regards to predictive models for hardness and reverse plasticity.

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1. Introduction

In a recent paper (Gerberich et al., 2003a), we demonstrated that the loading of single crystal silicon nanospheres produced hardnesses in the vicinity of 10 to 60 GPa. These were generally harder than bulk silicon single crystals. This was attributed to the high level of plastic strain and thus work hardening experienced by these very small volumes. The high hardnesses were achieved by sequentially loading each nanosphere to higher and higher loads thus increasing the internal defect structure. Along with their superhard character, these silicon nanospheres with radii from 19 to 46 nm exhibited reversed plasticity. This was theorized to occur because of the large internal stresses that develop when emitted dislocations at the top and bottom of the sphere contact nucleate and move down or up a glide cylinder. In nanoparticles, it requires relatively few dislocations to be emitted before they are only several nanometers apart representing high internal stresses. Because those high internal stresses can exceed the Peierls barrier, when the external load is removed, the dislocations retrace their paths and cause reverse plastic deformation. As pointed out in the previous study (Gerberich et al., 2003a), such reverse plastic deformation effects had been observed by Schaefer et al. (2003), Lilleodden et al. (1995), Kramer et al. (2001) experimentally; and by Yamakov et al. (2001) and Miller et al. (2004) with atomistic modeling. In the most recent paper (Gerberich et al., 2003a), an attempt was made to document this in terms of a reverse plastic strain with data for two nanoparticles. In doing so a cumulative displacement discrepancy, \( \delta_{CD} \), was measured. That is, when you loaded and unloaded one of these nanoparticles, an instantaneous residual displacement was measured. You could then reload the same nanosphere again and record the additional residual displacement. All of these residual displacements when summed together should be the total plastic displacement. When these are then subtracted from the original sphere height, they should equal the final height of the sphere. In fact there was a discrepancy for every nanosphere that experienced these multiple load–unload cycles implying that reverse plastic strain had occurred. The concept was that on immediate unloading the dislocations had little time to retrace their pathways so that the residual displacement indicated the plastic displacement under load. However, some time lapsed prior to the next run when the sphere heights were measured. The small probe scanning stresses combined with the larger internal stresses allowed a thermally activated, time dependent recovery process to take place. This phenomena was documented by defining a
cumulative displacement discrepancy, $\delta_{\text{CD}}$. This was measured as the difference between the summed residual displacements, $\sum \delta_{R_i}$, for all runs to the $i$th one and the change in the height of the nanoparticle measured after the $i$th run, $2r_i$, giving

$$\delta_{\text{CD}} = \sum \delta_{R_i} - (2r_0 - 2r_i).$$

(1)

It is clear that if there were no errors in measurement, the sum of the residual displacements for the $i$th run should be the difference in height between the initial particle, $2r_0$, and that measured for the $i$th run, $2r_i$. For perfect measurements and no reverse plastic strain, $\delta_{\text{CD}}$ should be zero. However, for the larger displacements in virtually all particles, $\delta_{\text{CD}}$ was found to be positive indicative of reverse plastic strain. While this was documented by Gerberich et al. (2003a) for two nanospheres, there was no analytical description of the process. In the present study this is quantified to first order recognizing the uncertainties in both the nanosphere slip plane orientation to the load axis and the severe limitations in the model which among other things does not account for the effect of image forces or for the non-uniformity of the stress distribution. With regard to not including image forces in the model, Liu et al. (2000) has shown that dislocation structures can be accurately predicted in free-standing nanoscale structures even when neglecting image forces since dislocation-dislocation interactions dominate. The model is then compared to both hardness measurements and the observations of reverse plastic displacement in individual load–displacement runs for nanospheres of different initial diameters. This model is partly based upon recent length scales proposed for explaining the indentation size effect (Gerberich et al., 2002) and thin film deformation and fracture (Gerberich et al., 2003b).

2. Experimental results and discussion

The experimental procedures for depositing, detecting and nanoindenting single crystal nanospheres are detailed by Gerberich et al. (2003a). To summarize those procedures, a hypersonic plasma particle deposition process described by Neuman et al. (1998) was utilized to produce a focused particle beam by using a series of aerodynamic lenses. This beam was deposited as a line onto a sapphire substrate and, simultaneously, part of the particle beam was collected onto a copper grid covered by a thin carbon film. Transmission electron microscopy of one of the collected nanoparticles is shown in Fig. 1. The contrast at the particle’s edge are thickness fringes and the diffraction and X-ray analyses indicated this to be a silicon single crystal. This and many other TEM images indicate these particles to be generally free of line or planar defects such as dislocations, twins and stacking faults.

Such defect-free single crystal nanospheres were located at the edge of a deposited line and imaged before and after nanoindentation with a 1 $\mu$m diameter diamond tip of an atomic force microscope (AFM) based nanoindenter. The before and after images of a 92.3 nm diameter particle subjected to a 15 $\mu$N normal force
are shown in Fig. 2(a) and (b). It is seen that the nanosphere has been vertically displaced 6 nm representing a 6.5% plastic strain as defined by $\delta/2r$. On a somewhat smaller 50.3-nm diameter nanosphere, six repeat load–displacement curves were conducted as seen in Fig. 3. As discussed elsewhere (Gerberich et al., 2003a), after each run the nanosphere increased in hardness. On the $x$-axis, a residual displacement, $\delta_R$, is seen to occur after each run representative of plastic deformation. These residual displacements are 1.5, 5.1, 7.2, 8.3 and 8.3 nm for the first five runs. As these total to 30.4 nm, the nanosphere should have only been 19.9 nm high after the fifth run but was measured to be 37 nm high. If the latter is a true
measure, then the sphere was only permanently reduced by 13.3 nm. This 17.1 nm displacement discrepancy (37–19.9) is a reverse displacement, \(d_{\text{rev}}\), attributed to reverse plastic strain. Based upon \(d_{\text{rev}}/2r\), the cumulative reverse plastic strain which occurred was 34%.

To discover the source of this reverse plastic strain, a number of possibilities were considered including amorphization and phase transformations under high pressure. In the previous study we had shown that atomistic simulations of even smaller nanospheres 12 nm in diameter did show amorphization but concluded that the simulation was on too small a volume to establish whether this might be a significant contributor to displacement. On unloading the atomistic simulations did not indicate any reversion to the crystalline phase so this was not considered as a possible mechanism. Regarding phase transformations, neither the loading nor the unloading curves were indicative of the type of pop-out phenomena that has been associated with the \(\beta\)-Sn phase transformation of silicon under high pressure. Corroborating experiments by Minor et al. (2005) involving in situ nanoindentation of thin silicon wedges in the transmission electron microscope confirmed that no amorphization or phase transformations had taken place. As we had postulated (Gerberich et al., 2003a), they also concluded that the observed nucleated dislocation loops were responsible for room temperature plastic deformation of silicon in these small
volumes. It should be pointed out that the dislocation loops they imaged and the prismatic loops we inferred from plastic deformation were both in relatively unconstrained samples. Thus, the triaxial pressure favoring phase transformations was not so great as in standard planar indentation experiments. To summarize these initial observations, we concluded that dislocation plasticity was the main, if not the only contributor to both permanent and reverse plastic deformation of the compressed nanospheres.

Even after the initial hypothesis, we wanted further verification of how reverse plastic displacement might be taking place. For that purpose we examined the earliest stages of deformation of a 38.6 nm diameter nanosphere repeatedly loaded

Fig. 4. The first, fourth, eighth and ninth load ($P$) vs. displacement ($\delta$) curves for a silicon nanosphere with an initial measured height of 38.6 nm. It is thought that upon loading the forward steps represent dislocation nucleation; while upon unloading the reverse steps are associated with dislocation annihilation and/or cross-slip with free surface emergence.
nine times. The first, fourth, eighth and ninth runs are shown in Fig. 4. The first striking feature is that, except for the first run to 4.8 μN, there were both forward steps on loading and backward steps on unloading. The second striking feature was that for the first run the cumulative displacement of all of the steps equaled the residual displacement on unloading. The third striking feature was that nearly all steps were equal to about 0.2 nm close to the 0.236 nm displacement associated with a Burgers vector in silicon. The fourth striking feature was that substantial unloading occurred prior to a backward step. Our interpretation is that the forward steps are associated with dislocation nucleation while the backward steps are associated with annihilation and/or cross-slip with free surface emergence. This is consistent with the two-dimensional simulation of forward and reverse dislocation reaction shown by Miller et al. (2004) in single crystal thin films of aluminum. For Fig. 4(a) it is believed that the generated internal stresses were insufficient to cause reverse plasticity. Subsequent runs did produce backward steps. First, it is suggested that these backward steps of burgers vector character are not what might be expected if a reverse phase transformation occurred. Second, it is seen that the relative number of steps appears to diminish compared to the residual displacement after unloading. In Fig. 4(a) all residual displacement can be accounted for by steps while in Fig. 4(b) only 52% of the displacement is accounted for by steps. That is, we count the forward steps (1.35 nm) and subtract the backward steps (0.6 nm). If only steps were involved, the net residual displacement would be (1.35−0.6) 0.75 nm. However, 1.65 nm of displacement is measured on unloading suggesting that only half of this residual displacement is accounted for by dislocation nucleation. This was further examined for all nine runs to ascertain how much residual plasticity was generated by dislocation nucleation as exhibited by steps in the \( P–\delta \) curves. The difference in localized plasticity is discussed using Fig. 5(a) where concentric loops moving up or down a glide cylinder during loading and unloading is illustrated. If the loops are nucleated on loading and are annihilated or emerge out of the free surface on unloading these could lead to steps. On the other hand if pre-existing dislocations are moved further under higher loads and shear stresses, the displacement may vary more smoothly. By summing the displacements associated with all steps (forward–backward) and dividing by the residual displacement found on unloading for each run, we have a good estimate of the fraction of plasticity associated with net dislocations nucleated or annihilated. For the nine runs under increasing load this is shown in Fig. 5(b). It is seen that the steps account for the early deformation in the relatively dislocation-free sphere but that later on the same sphere appears to have more of its residual plasticity associated with moving pre-existing dislocations. While this is highly speculative it does appear that a change in the details of the deformation mechanism takes place during repeated cycling of the same nanosphere.

From the above results and discussion we conclude that dislocations are the primary source of plasticity. Furthermore, due to large internal stresses some reverse plasticity takes place by dislocations moving backwards and/or annihilating. Ignoring some of the above detailed observations so as to arrive at a first order description of reverse plasticity we only consider dislocation nucleation and
Fig. 5. (a) Idealized schematic of the compression of a nanosphere where concentric dislocation loops are shown moving up or down a glide cylinder during loading and unloading. The fraction of the summed step displacement divided by the total residual displacement for each of the nine indentation runs is shown in (b). Steps account for the deformation in the initial compressions whereas after the fourth run, the majority of the deformation is associated with moving previously nucleated dislocations.
disappearance. The latter are assumed to result by free surface emergence or annihilation. Next, two simple analytical models, one for reverse plasticity and one for hardness are developed and compared to experimental observations.

3. Analytical models

Based on Fig. 5(a) the spacing between edge dislocations under load at a shear stress, $\tau_{\text{flow}}$, arranged along a glide cylinder would be given by Hirth and Loethe (1982) as

$$x_s^L = \frac{\mu b}{2\pi(1-\nu)\tau_{\text{flow}}},$$

where $\mu$ and $\nu$ are the shear modulus and Poisson’s ratio and $b$ is the burgers vector. When the external load is released, it is assumed that the high internal stress causes dislocations to retrace their path until the Peierls barrier stops them. The spacing under no load, ignoring image forces, would be

$$x_s^U = \frac{\mu b}{2\pi(1-\nu)\tau_{\text{p}}}. \quad (3)$$

Under an applied shear stress, the number of dislocations created as an inverse pile-up as taken from Eshelby et al. (1961) is

$$N = \frac{\pi(1-\nu)\tau_s}{\mu b}, \quad (4)$$

where we treat $\ell_s$ as the length scale of the deformation process. As dislocation loops nucleate and move up or down a glide cylinder, each inverse pile-up at the top and bottom may have $N$ dislocations given by

$$N = \frac{\delta}{2b}, \quad (5)$$

where half the displacement, $\delta$, is at the top and half at the bottom. We define the load, $P$, in terms of the shear stress times the contact area multiplied by an appropriate factor representative of the state of stress and the orientation of the slip plane and slip vector. It might be two for uniaxial compression and six for fully constrained plastic indentation. Because of the uncertainties, we choose an intermediate value of four. Since the geometric contact area as used by Gerberich et al. (2003a) is given by $a^2 = \delta r - \delta^2/4$, this gives the load as

$$P = 4\pi a^2 \tau_{\text{flow}} = 4\pi \tau_{\text{flow}} \left(\delta r - \frac{\delta^2}{4}\right). \quad (6)$$

With (2), (4), (5) and (6), the number of dislocations under load at the top and bottom is given by

$$N_L = \frac{\ell_s P(1-\nu)}{2\mu b \left(\delta r - \frac{\delta^2}{4}\right)}.. \quad (7)$$
Similarly, the number of dislocations after unloading at the top and bottom is given by

\[ N_U = \frac{2r}{x_U} = \frac{2\pi(1 - \nu)(2r - \delta)\tau_p}{\mu b}. \]  

Clearly, if \( N_L > N_U \), some dislocations must retrace their paths or annihilate. Ignoring image forces, this reverse displacement would be with (7) and (8)

\[ \delta_{\text{rev.}} = (N_L - N_U)b = \left( \frac{(1 - \nu)P\ell_s}{2(\delta r - \delta^2/4)\mu} - \frac{2\pi(2r - \delta)(1 - \nu)\tau_p}{\mu} \right). \]  

Defining \( \ell_s \) as a volume to surface ratio as used by Gerberich et al. (2002, 2003a,b) for the top and bottom contacting surfaces of a sphere, this becomes

\[ \ell_s = \frac{V}{S} = \frac{2r^2}{3\delta}. \]  

If this could be documented, then it is a simple insertion of (10) into (9) to give

\[ \delta_{\text{rev.}} = \frac{(1 - \nu)}{\mu} \left( \frac{P\ell^2_s}{3(\delta^2 r - \delta^3/4)} - 2\pi(2r - \delta)\tau_p \right). \]

4. Results and discussion

To first address the usefulness of (10), we demonstrate that combined with (7) this does give a first order prediction of the hardness variation with increased displacement depth. With (5), (7) and (10) it is seen that

\[ P = \frac{3\mu\delta^2(\delta r - \delta^3/4)}{2r^2(1 - \nu)}. \]  

Furthermore, hardness is defined as \( P/\pi a^2 \) and as before \( a^2 = \delta r - \delta^2/4 \) for geometric contact. With (12) these give

\[ H = \frac{3\mu}{(1 - \nu)2\pi} \left( \frac{\delta}{r} \right)^2. \]  

In a current investigation however, we demonstrate that there are two terms associated with hardness when probing very small volumes of nanospheres or films (Jungk et al., 2004). At the smallest displacement there is a term associated with surface energy and a second term at deeper depths associated with a dislocation back stress. In that paper we find

\[ H = \frac{7}{8} \tau_{ys} \left( \frac{\ell^2_s}{\delta r} \right)^{1/3} + \frac{3\mu}{2\pi(1 - \nu)} \left( \frac{\delta}{r} \right)^2. \]
Since $V/S$ or $\ell_s$ can also be given as $2r^2/3a^2$ and $a^2 \sim \delta r$ to first order, we find for the first term of Eq. (14) that
\[
\left( \frac{\ell_s^2}{\delta r} \right)^{1/3} = \left( \frac{r^6}{a^6} \right)^{1/3} \left( \frac{2}{3} \right)^{2/3} = \left( \frac{r}{a} \right)^2 \left( \frac{2}{3} \right)^{2/3}.
\] (15)
Again, invoking $a^2 \sim \delta r$ and combining (14) and (15) leads to a very simple relationship for hardness given by
\[
H = \frac{2}{3} \sigma_{ys} \left( \frac{r}{\delta} \right) + \frac{3\mu}{2\pi(1-v)} \left( \frac{\delta}{r} \right)^2.
\] (16)
Experimentally, we find for these nanospheres that the hardness is quite high at the smallest of displacements, goes through a minimum and then continues to harden as the internal stresses and/or pressures develop at very large displacements. This is analogous to an initial indentation size effect followed by a dislocation hardening effect for thin films.

From observed hardness minimums, we can find a yield strength appropriate to the best data fit for a given displacement of a given radius nanosphere. Differentiating (16) we find the displacement at the hardness minimum to be
\[
\delta_{H_{\text{min}}} = r \left( \frac{2\pi \sigma_{ys}(1-v)}{9\mu} \right)^{1/3}.
\] (17)
For the 50.3 and 92.7 nm diameter nanospheres we find experimental minima at 8 and 11 nm, respectively. From (17) one can immediately see that since $\delta/r|_{H_{\text{min}}}$ is larger for the smaller nanosphere that there is a size dependent $\sigma_{ys}$. We find $\sigma_{ys}$ equal to be 9.7 and 4.0 GPa for these two nanospheres with the corresponding data fits shown

![Diagram](image)

Fig. 6. Hardness vs. displacement for 50 and 93 nm diameter nanospheres compared to (16) with $\sigma_{ys}$ = 9.7 and 4.0 GPa for the smaller and larger particles, respectively.
in Fig. 6. Similar determinations were made for the other nanospheres resulting in no unknowns for (16). For silicon, the coefficient of $3\mu/(1 - \nu)2\pi$ in (16) is 41.5 GPa. Reasonable data fits for the 38.6 and 43.6 nm diameter nanospheres were also found in this manner resulting in $\sigma_{ys}$ values of 17.7 and 14.9 GPa, respectively. It seems then that the smaller the nanoparticle the higher the yield strength.

With this demonstration, we judged it realistic to use (11) to assess reverse plastic flow. As one might anticipate there is tremendous scatter for an individual load displacement curve. When subtracting a small residual displacement from an equally small height measurement of a sphere, the error may be compounded. Experimentally, the spheres would have to deform symmetrically and one would have to be at the same apogee for each measurement. Data for all nanoparticles are shown in Fig. 7. For curve fitting, the only unknown in (11) for a given sphere radius, $r$, loaded to a specific load and displacement $(P, \delta)$ is the Peierls stress, $\tau_p$. For three general groupings of nanoparticles we calculated curves in Fig. 7 representing average Peierls stresses of 1.6, 5.5 and 8.5 GPa for the large, medium and smallest nanoparticles, respectively. While the data were very scattered as expected, the general trends represented by (11) were followed. Physically, the rationale is that the larger loads representative of greater internal stresses due to more closely spaced dislocations results in larger reverse plasticity at the largest cumulative strains. At the smallest strains, again the reverse plasticity is predicted to be greater than the minimum because of the length scale used at (10). This surface dependent effect may in fact be associated

![Fig. 7. Reverse displacement upon unloading as a function of cumulative plastic strain represented by $\delta_{cum}/2r$. The curves are from (11) representing three general nanosphere sizes.](image)
with a strong image force even though this was not explicitly involved in the derivation. It should be noted here that the modulus of SiO$_2$ is considerably less than Si allowing for the image force to draw dislocations toward the free surface.

One final comparison was that of how nanosphere size and deformation level affected yield stress and hardness. For that purpose we took each set of individual nanoparticle data and calculated a $\tau_p$ for the best average data fit from (11). This was then compared to the $\sigma_{ys}$ as obtained from (16) and (17) and reported above. The comparison in Table 1 assumes that $\sigma_{ys} \sim 2\tau_p$. To first order this does appear to be the case. It is also seen that the Peierls and yield stress decrease rapidly with increasing nanosphere radius. It should be noted that this increase in strength with decreasing length scale is much greater than what might be anticipated from a Hall-Petch relationship which would predict a $d^{-1/2}$ dependence.

Regarding hardness, we see that the second term of (16) has a strong displacement dependence. Clearly then, while the Peierls and yield stresses may be intrinsically higher for the smaller particles, there also should be an increasing dependence with larger strain. Large strain at large load will be accompanied by large pressures. There is then a question as to what happens to the flow stress of these nanoparticles as we increase load. We had previously assumed that they simply work-hardened (Gerberich et al., 2003a). However, recent atomistic simulations on Ta by Moriarty et al. (2002) showed that both the hardness and hence the Peierls barrier as well as modulus of elasticity increased at large pressures. To explore this further we decided to determine the hardness to modulus ratio from a relationship developed by Cheng and Cheng (1998). From the ratio of work of indentation during unloading, $W_U$, to the total work of indentation to maximum load, $W_{tot}$, one can find

$$\frac{H}{E^*} \cong \pi_0 \left(1 - \frac{W_U}{W_{tot}}\right),$$

where $\pi_0$ is a function of material properties. To first order, however, for a wide range of hardening characteristics and different materials Cheng and Cheng (1998) found $\pi_0$ is nearly constant. Since $H/E^*$ decreased linearly with the term inside the brackets, this gave

$$\frac{H}{E^*} \approx 0.22 \frac{W_U}{W_{tot}}.$$  \hspace{1cm} (19)

By integrating areas under all experimental load–displacement curves for the nine sets of data like those in Fig. 4, we determined $W_{U}/W_{tot}$. For reference $W_{tot}$ ranged from $5 \times 10^{-15}$ to $9 \times 10^{-14}$ Nm as load increased from 5 to 30 $\mu$N as seen in Fig. 8. Thus, work increased by a factor of 18 while load increased by a factor of six. Values

<table>
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<th>Sphere radius (nm)</th>
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<th>22</th>
<th>25</th>
<th>32</th>
<th>46</th>
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<tbody>
<tr>
<td>$\sigma_{ys}$ (GPa)</td>
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<td>14.9</td>
<td>9.7</td>
<td>–</td>
<td>4.0</td>
</tr>
<tr>
<td>$2\tau_p$ (GPa)</td>
<td>17.0</td>
<td>9.0</td>
<td>13.0</td>
<td>3.4</td>
<td>3.0</td>
</tr>
</tbody>
</table>

Table 1
Comparison of $\sigma_{ys}$ as obtained from Eqs. (16) and (17) to $2\tau_p$ as obtained from fitting (11)
of $W_t/W_{tot}$ ranged from 0.42 down to 0.22. With Eq. (19), the corresponding values of $H/E^*$ are shown in Fig. 8 as a function of increasing load. For loads up to 20 μN, representing a strain of about 0.2, both $W_{tot}$ and $H/E^*$ were well-behaved. It is seen that $H/E^*$ is nearly constant suggesting that hardness tracks modulus as found in the τp simulations at high pressure. However, at even higher loads $H$ starts decreasing with respect to modulus in Fig. 8. One could interpret that as a relative decrease in hardness or a relative increase in modulus. We tend toward the former explanation since the displacement range is in the early part of $H$ vs. $\delta$ curve shown in Fig. 6. Irrespective of what mechanism is leading to a change in the hardness/modulus functionality, it seems that at least two mechanisms are involved in the overall hardening process associated with nanoparticle deformation.

5. Summary

In summary, we have shown that reverse plastic displacement occurs in highly strained nanospheres of silicon. With strain defined as cumulative displacement normalized on sphere diameter, it is found that reverse displacement tends to go through a minimum with increasing strain. This is predicted to first order by a simple model which addresses the number of dislocations at equilibrium under load and no-load conditions. In addition, hardness goes through a minimum and the several possible explanations given are under current investigation.
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References


