Abnormal stress drop at the yield point of aluminum nanowires: A molecular dynamics study

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Molecular dynamics (MD) and experimental data indicate that the stress at the yield point of uniaxially stretched nanowires suffers a sudden large drop (D). In addition, nanowires show a yield strength (YS) significantly higher than that of bulk material. In this work, aiming to identify the parameters characterizing the nanowire that produce these effects, MD simulations are carried out at low temperature (0.5 K) on defect-free aluminum nanowires stretched along the (100) direction. Nanowires are characterized by the aspect ratio and the average coordination. The results can explain neither the absence of the drop in bulk material nor its much lower YS: both yield strength and drop increase logarithmically with the aspect ratio and linearly as the average coordination tends to its bulk value. Increasing the testing temperature smoothes the stress-strain curve and significantly reduces the YS, but does not eliminate the drop whose relative value D/YS remains practically constant. Introducing vacancies reduces both the yield strength and the drop. A detailed analysis of the atomic positions reveals a strong necking at the yield point of defect-free nanowires (absent when vacancies are introduced) that may surely be the cause of the drop.

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I. INTRODUCTION

Mechanical properties of nano-scale systems is one of the fields in the area of nanoscience that is increasing most rapidly.[1–19] Apart from the obvious size dependence of mechanical moduli,[7,14] recent experiments and numerical simulations have identified two features in the stress-strain curve that do not occur in macroscopic solids. We refer to the absence of hardening[6,9,12,16,17] and to a drop of the stress at the yield point observed in experiments[20] and numerical simulations.[8,12,14,16–18] Moreover, nanowires have an unusually high yield stress, almost an order of magnitude higher than that of bulk material.[8,14,18]

Concerning hardening, it is widely accepted that as soon as the system becomes smaller than the characteristic length of nucleation and/or interaction among dislocations,[21,22] no hardening is expected, a result confirmed by several numerical simulations,[12,16,17] albeit experiments, however, have not yet given an unambiguous answer.[16] As regards the stress drop at the yield point, extensive molecular dynamics (MD) on copper,[14,18] aluminum,[16,17] and gold[8,17] nanowires clearly demonstrate its existence; moreover, experiments on rather thin gold wires do also indicate the presence of the drop.[20] Although the origin of this drop may be related to that of the unusually high yield strength, namely the reduction in dislocation activity due to the small cross section of the nanowire,[8] it is pertinent to carry out further studies of this issue.

In this work we present MD calculations aiming to identify the parameters which, characterizing size and shape of the nanowires, are responsible for that stress drop. In particular aluminum nanowires will be stretched at constant strain rate and constant temperature. The nanowires are characterized by the aspect ratio A and the average coordination C (this is more accurate than the fraction of surface atoms S) whose size and shape were varied in such a way that the two variables A and C varied separately, unlike in previous studies.[10]

The results show that, over the range covered here, the stress drop D varies logarithmically with the aspect ratio, as the Young modulus (Y) and the yield stress (YS) do, while the three magnitudes increase linearly with C. These results indicate that only Y behaves as expected, namely increasing C should lead those magnitudes to reach their bulk value, in particular $D = 0$ in bulk material. Having checked that neither YS nor D behave as expected when the nanowire geometry or size is changed, we investigate the effects of vacancies concluding that they produce the effect we were looking for, namely they eliminate the drop and reduce the YS.

The rest of the paper is organized as follows. Details of the MD simulations are presented in Sec. II, where the expressions used to calculate the average coordination and the stress tensor are given. The section devoted to the results (Sec. III) starts with a brief discussion of the characteristics of the stress-strain curve in defect-free nanowires. Next, numerical results for the Young modulus (Y), yield strength, and drop of defect-free nanowires having different aspect radii and average coordination are presented and discussed. Sec. III A starts with a brief discussion of the effects of the testing temperature on the stress-strain curve and once checked that, as in the case of size and geometry, it cannot be responsible of the absence of the drop in bulk material, the effects of vacancies are discussed in detail. Section IV is devoted to the conclusions that emerge from the present work.

II. METHODS

MD calculations were carried out on Al nanowires stretched along the [001] direction at a rate of 0.01 Å per picosecond which for nanowires of length 5–50 Å, gives a strain rate of

$\dot{\epsilon} = 2 \times 10^8$–$2 \times 10^9\ s^{-1}$. This rate is far above that commonly used in experiments, 0.1–1 s^{-1}, although values as high as $10^4\ s^{-1}$ and as low as $10^{-4}\ s^{-1}$ can also be found in current literature. Unfortunately, no MD simulation can be performed at such low strain rates.[23] As initial conditions we took fixed atomic positions in a perfect fcc lattice and the velocity at each atom randomly distributed. The interatomic potential used in the simulations was taken from Ref. 24. Simulations were done on single crystal nanowires of two different shapes: (i) parallelepipedic nanowires of dimensions $m \times m \times n$ (see Table I), where m and n are given in units of the interatomic distance (2.86 Å in Al), and (ii) samples of cross section decreasing from the edges to the center.[16,17,19] Moreover, in most calculations the testing temperature was fixed at 0.5 K, which amounts to assume that the nanowire is in thermal contact with a bath large enough to absorb all heat generated along stretching. The latter was implemented by rescaling all atom velocities every 10 MD steps.[25,26] Some results obtained at temperatures up to 200 K will be also presented.

Stretching along the [001] direction was carried out by displacing and fixing the one and half layers of the unit cell at one end of the nanowire and only one at the other end. This ensures that the portion of the nanowire containing only mobile atoms, i.e., atoms that are allowed to move freely in the simulation, is bounded by the same type of plane. The displacement applied to the fixed atomic layers is 0.01 Å every ps. Although the results presented here correspond to a single realization (initial distribution of atomic velocities) we have checked that they do not significantly depend on the particular realization (see below). Y was calculated averaging over the whole elastic range (note that weak deviations from the linear relationship between stress and strain that characterizes the elastic range cannot be discarded).

TABLE I. Young modulus Y, yield stress YS, and drop at the yield point D (all in GPa) in Al nanowires subjected to constant strain rate stretching. The nanowire dimensions are $m \times m \times n$, where n is the stretching direction (the reason while n is half-integer is explained in the main text). N_a is the number of mobile atoms, $S = 1/m$ approximately gives the ratio of surface to bulk atoms, $A = n/m$ is the aspect ratio, and C is the average coordination of mobile atoms.

Nanowire	A	S	N_a	C	Y	YS	D
$10 \times 10 \times 2.5$	0.25	0.1	1000	9.24	32.5	2.37	1.02
$10 \times 10 \times 4.5$	0.45	0.1	1800	9.72	37.4	2.92	1.30
$10 \times 10 \times 7.5$	0.75	0.1	3000	9.99	44.7	3.60	2.18
$10 \times 10 \times 10.5$	1.05	0.1	4200	10.1	50.0	4.13	2.71
$10 \times 10 \times 13.5$	1.35	0.1	5400	10.2	52.9	4.61	3.00
$10 \times 10 \times 15.5$	1.55	0.1	6200	10.2	52.9	4.85	3.13
$10 \times 10 \times 17.5$	1.75	0.1	7000	10.2	56.2	5.11	3.87
$10 \times 10 \times 19.5$	1.95	0.1	7800	10.3	52.9	5.30	3.30
$10 \times 10 \times 23.5$	2.35	0.1	9400	10.3	61.9	5.64	4.57
$5 \times 5 \times 2.5$	0.5	0.2	250	8.2	28.4	2.39	0.94
$9 \times 9 \times 4.5$	0.5	0.11	1458	9.7	38.9	2.94	1.28
$13 \times 13 \times 6.5$	0.5	0.077	4394	10.3	49.3	3.30	1.44
$15 \times 15 \times 7.5$	0.5	0.067	6750	10.5	48.6	3.40	1.71
$19 \times 19 \times 9.5$	0.5	0.053	13718	10.8	51.1	3.59	2.10
$23 \times 23 \times 11.5$	0.5	0.044	24334	11.0	57.1	3.70	1.98
$31 \times 31 \times 15.5$	0.5	0.032	59582	11.3	62.1	3.78	1.96

We characterize the shape and size of the nanowires by means of the aspect ratio $A = n/m$ and the average coordination C (see Table I). The latter is defined as

$$C = \frac{1}{N_a} \sum_{i=1}^{N_a} N_{nn}(i), \tag{1}$$

where N_a is the number of mobile atoms in the nanowire and $N_{nn}(i)$ is the number of nearest neighbors of atom i considering an interatomic distance of 2.86 Å. The ratio of surface to bulk atoms, approximately given by $S = 1/m$, is also reported in Table I. We choose nanowires having either C varying over the range 8–11 and a constant aspect ratio $A = 0.5$ or an aspect ratio varying in the range 0.25–2.35 while keeping C as constant as possible (actually it varies in the narrow range 9–10, see Table I).

The stress tensor can be easily derived from molecular dynamics calculations as,[26]

$$\sigma_{\alpha\beta} = \frac{1}{V} \left(\sum_{i=1}^{N} m_i v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{i \neq j}^{N} r_{ij\beta} F_{ij\alpha} \right), \tag{2}$$

where V is the volume of the sample, $v_{i\alpha}$ is the component α of the velocity vector at atom i, $r_{ij\beta}$ is the component β of the vector that joins atoms i and j, and $F_{ij\alpha}$ is the component α of the force that atom i exerts on atom j. As seen in Eq. (2) both the kinetic and the potential energy contribute to the stress tensor [the first and second terms in the right-hand side of Eq. (2)]. Calculations have been done replacing V at each instant by its initial value. This gives what is known as engineering stress. Accordingly, we have used the increment in length divided by the initial length as a variable to characterize deformation, known as engineering strain. We have checked in a few cases that the results do not qualitatively change if the instant volume is introduced in Eq. (2). If the external force is applied in the z direction, the stress is given by σ_{zz} in Eq. (2).

III. RESULTS

A. The stress-strain curve of defect-free nanowires

Stress-strain curves for three Al nanowires either with very different A and similar C (a) or the same A and very different C (b) are shown in Fig. 1. Beyond the yield point, the quasielastic events followed by sudden drops of the total stress, associated to major atomic rearrangements[5,12,16,27] are clearly seen. Concomitantly with the decrease in D, as the aspect ratio A decreases, there is a sharp reduction in the abruptness of the drop. The experimental stress-strain curve reported in Ref. 20 for a thin gold wire (a wire characterized by a conductance of 50 quanta and, thus, 50 atoms in its narrowest cross section) is similar to some of those reported here and in Ref. 12.

Figure 2 illustrates how the stress drop at the yield point depends on the initial conditions (realization). The standard deviation of the drop D is 8%. The standard deviation in the Young's modulus and the yield stress is much smaller. The results were obtained on nanowires of variable cross section and containing 463 atoms, such as those used in Ref. 17.

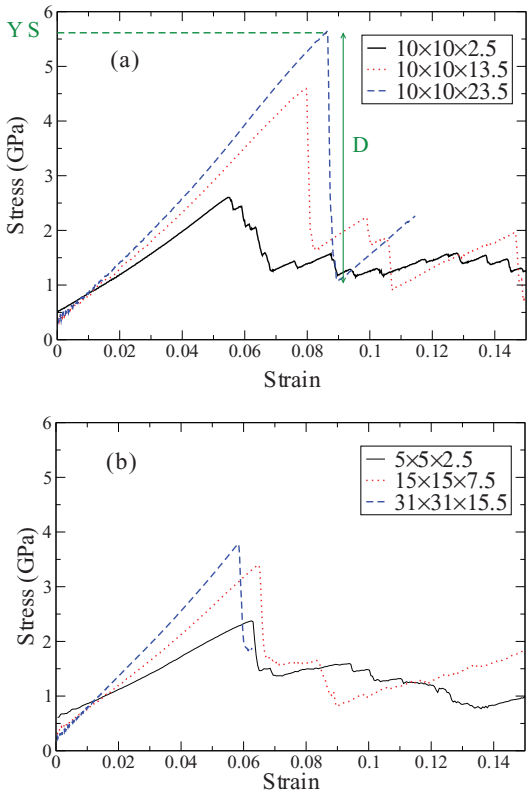
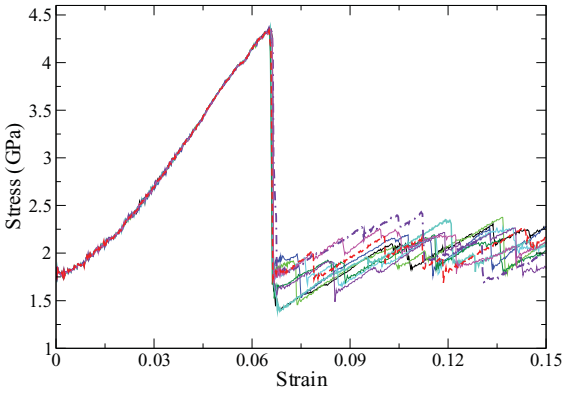


FIG. 1. (Color online) Engineering stress versus engineering strain in aluminum parallelepipedic nanowires. (a) Nanowires having a similar average coordination C and a very different aspect ratio A (see Table I). (b) Nanowires with the same aspect ratio and a rather different C. The results correspond to a single realization (initial distributions of atomic velocities). The yield stress YS and the drop D at the yield point are indicated.

B. The Young modulus, yield stress, and stress drop in defect-free nanowires

Table I reports numerical results for Y, YS, and D and a total of 16 nanowires having different A and C. Plots of those three magnitudes versus A and C are shown in Fig. 3. Note



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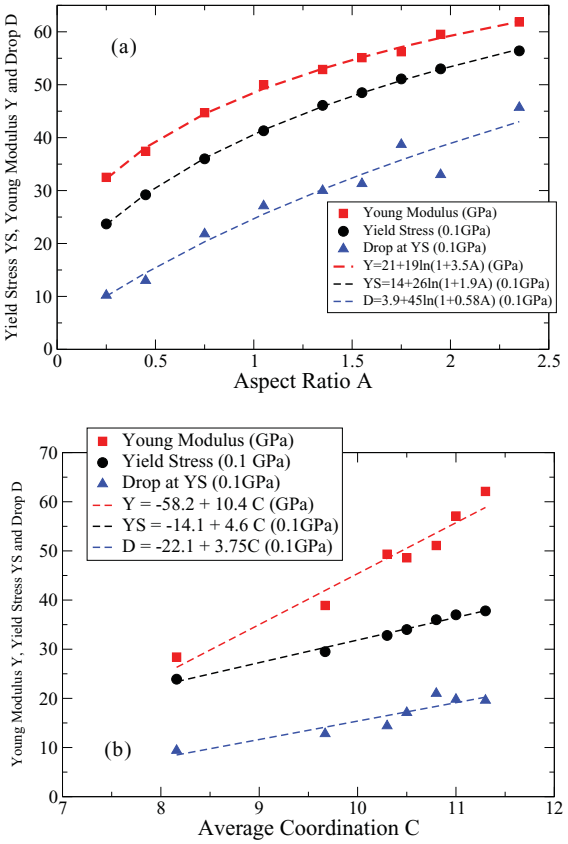

FIG. 3. (Color online) (a) Young modulus Y, yield stress YS, and drop in the engineering stress at the yield point D versus the aspect ratio A of nanowires having the same fraction of surface atoms S (0.1 see Table I) and a similar average coordination C (also shown in Table I). The results for the three magnitudes admit a fitting with a logarithm (also shown in the figure). (b) Y, YS, and D versus the average coordination C of nanowires having the same aspect ratio A (0.5, see Table I).

that while Y is of the order of magnitude of that found in bulk material, YS is at least an order of magnitude higher.[28]

As shown in Fig. 3(a), Y, YS, and D increase with A. The numerical results can be fitted by a logarithmic law, as suggested in Ref. 29 based on *ab initio* calculations on gold nanowires. The logarithmic law, inspired in the Hall-Petch relation for bulk materials, does probably hold over a limited range of values of A, as it is unlikely that for A tending to infinity Y does also tend to infinity as that law implies. In addition, the results reported in Ref. 29 indicate that there is a linear relationship between YS and Y. This was also observed here for both YS and D and with the same slope (see Fig. 4).

Numerical results for Y, YS, and D versus the average coordination C are depicted in Fig. 3(b). Now the three magnitudes increase linearly with C. It is noted that, in the bulk limit $C = 12$, the law fitted to the numerical data reported in Fig. 3(b) gives $Y = 66.6$ GPa, not far from the bulk value Ref. 28. On the other hand, YS and D behave just opposite to what is expected, as both should decrease as the bulk limit is reached; in particular, for $C = 12$, D should vanish. Again we should warn against extrapolating these fittings too far away from the fitting range. However, extrapolating up to the bulk value of C is in our opinion valid as the upper limit of the fitting

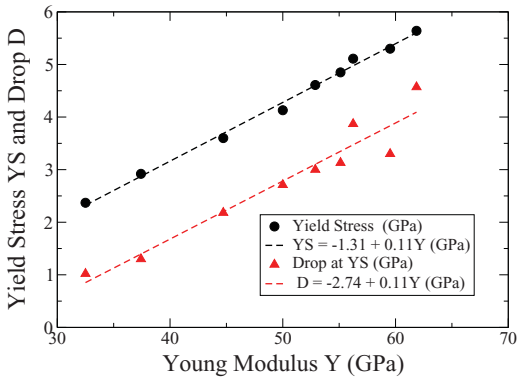

FIG. 4. (Color online) Yield stress YS (circles) and drop in the engineering stress at the yield point D (triangles), versus Young modulus Y of nanowires having the same fraction of surface atoms $S = 0.1$ (see table in main text) and a similar average coordination C. The results for the two magnitudes can be nicely fitted by straight lines with the same slope.

range already goes up to 11.3 (see Table I). We note that there is almost a linear relationship between YS and D [the slopes of the lines fitted in Fig. 3(a) are very similar], although in this case none of these magnitudes is linearly related with Y.

Several studies[10,11] investigate how Y varies as the nanowire diameter increases, keeping constant its length. In doing so, both A and C change. Actually, C varies appreciably when the nanowire cross section is changed and depends only slightly on length. Thus, it is not easy to compare the present results with those reported in Refs. 10 and 11. Anyhow, MD results[10] indicating that Y of Cu nanowires compressed along the [001] and [111] directions increase with the nanowire diameter tending asymptotically to its bulk value are compatible with those reported here (see Table I and Fig. 5). Compressing the wires along the [110] direction led to the opposite behavior, namely a decrease of Y with diameter.[10] On the other hand, bending experiments on non-oriented Ag nanowires[11] indicate that Y does decrease with the diameter tending to its bulk value

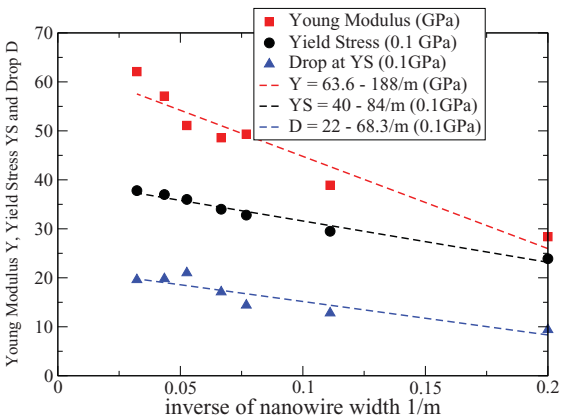

FIG. 5. (Color online) Young modulus Y (squares), yield stress YS (circles), and drop in the engineering stress (triangles) at the yield point D versus the inverse of the nanowire width m of nanowires having the same aspect ratio $A = 0.5$ (see Table I).

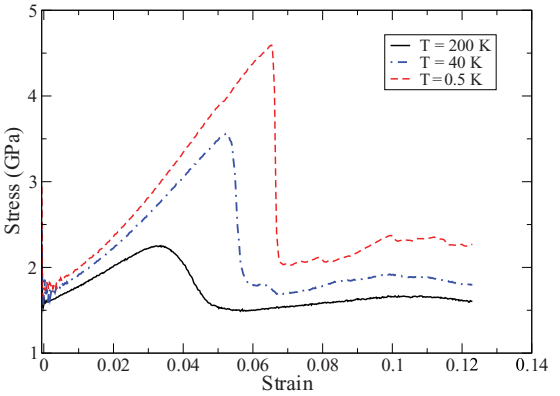

FIG. 6. (Color online) The stress drop at the yield point is not eliminated when the testing temperature is raised. As expected, increasing the temperature smoothes the stress-strain curve. Results obtained on nanowires of variable cross section and containing 463 atoms such as those used in those used in Ref. 17.

asymptotically, In addition, an expression for Y that includes surface effects was derived in Ref. 11,

$$Y = Y_b + \frac{1}{d}\left(8S + \frac{8}{5}\tau_0 A^2\right), \tag{3}$$

where $A = l/d$ is the aspect ratio, l and d being the nanowire length and diameter, Y_b is the bulk Young modulus, S is the surface modulus, and τ_0 the surface stress. When A is kept constant, the linear relationship between Y and $1/d$ also holds in the present case with $Y_b = 63.6$ GPa,[28] although with a negative slope, i.e., in our case Y increases as the nanowire diameter increases. This difference could be due to the fact that the samples used in the experiments[11] were not oriented while we stretched the nanowire along the [001] direction.

C. Effects of vacancies

The results just discussed indicate that neither shape nor size determine the stress drop. After having checked that raising the testing temperature, while it smoothes the stress-strain curve and reduces significantly the YS, does not diminish

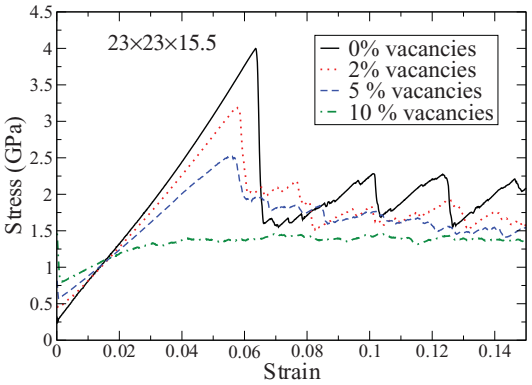

FIG. 7. (Color online) Engineering stress versus engineering strain as derived from MD calculations on Al $23 \times 23 \times 15.5$ nanowires containing several vacancies concentrations. The results correspond to a single distribution of vacancies.

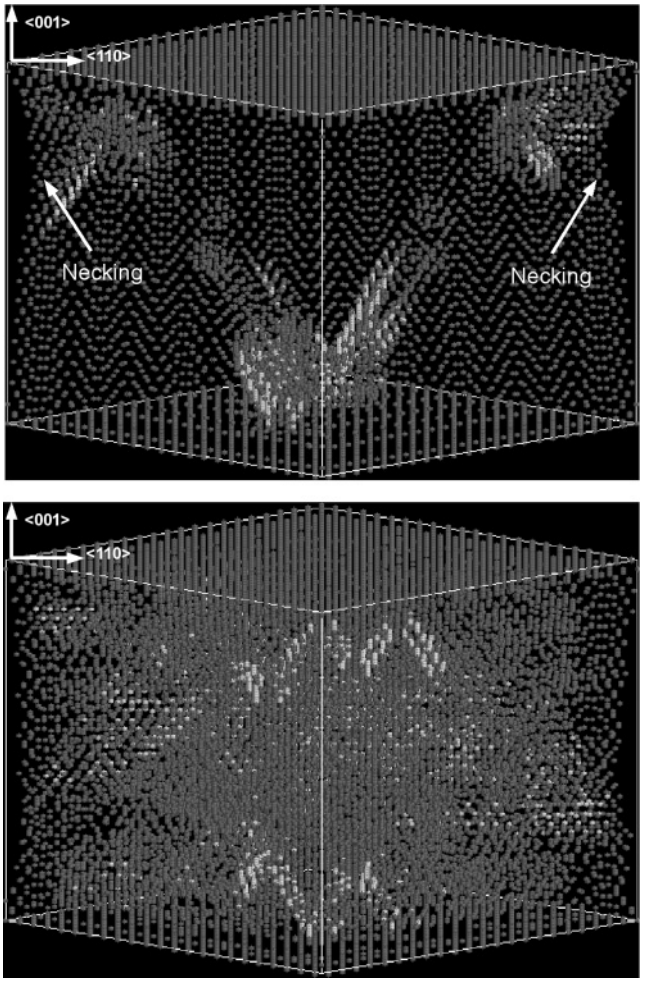

FIG. 8. (Color online) The atomic arrangement in a nanowire of dimensions $23 \times 23 \times 15.5$ (32798 mobile atoms) stretched along the [001] direction just after the drop at the yield point, without vacancies (upper) and with 5% vacancies (lower). Note the strong necking in the former case. Gray points denote atoms without an fcc environment (22069 and 8730 for nanowires with and without vacancies, respectively) while white points denote atoms having an hcp environment. As surface atoms do not have an fcc environment, they are also denoted by gray points. Atoms having an fcc environment are not shown.

the relative value of the drop D/YS (see Fig. 6), we have explored a factor essential to the plastic behavior of materials, namely, defects. In particular we have investigated the effects of vacancies, as extended defects such as dislocations are less likely in small systems. As shown in Fig. 7, vacancies strongly modify the stress-strain curves of a $23 \times 23 \times 15.5$ nanowire. Already a 2% of vacancies sharply reduces the YS and diminishes and smoothes the stress drop at the yield point. At high concentrations, vacancies eliminate the drop and, as a result, the stress-strain curve does not differ that much from those obtained in bulk material. As vacancies reduce the average coordination in the nanowire, we have calculated C in the four cases of Fig. 7, resulting in $C = 11.09$, 10.87, 10.55, and 10 for 0, 2, 5, and 10% vacancies. Comparing these results with those obtained on defect free nanowires depicted in Fig. 1(b) and Table I, we note that the effect of vacancies cannot be correlated with that of C.

In order to understand the mechanisms at the atomic level driving the drop at the yield point, we have computed the local environment of each atom to identify those defects produced during straining. The common neighbor analysis method[30] is used to classify atoms as fcc type (corresponding to perfect structures), hcp type (associated to stacking faults), and all other atoms (related to defects of different types). In doing so we used as a cut-off distance the interatomic distance in fcc aluminum.

Figure 8 shows the atomic arrangement just after the stress drop in nanowires with and without vacancies. It is clear from this figure that the perfect nanowire (upper illustration in Fig. 8) shows a strong necking as a result of the nucleation of dislocations at the surface. In view of these results, we can provide an explanation for the dependence of D and YS with average coordination and aspect ratio shown in Fig. 3. Both D and YS must increase with aspect ratio since the local stresses needed to nucleate a dislocation are achieved easier when the aspect ratio is smaller. Both D and YS also increase with coordination since the number of surface atoms is reduced and, therefore, the number of possible nucleation sites for dislocations is also reduced. On the other hand, Fig. 8 (lower panel) shows that a nanowire with 5% vacancies has a more uniform reduction of cross section. This reveals what the origin of the drop may be: Whereas the nanowire without vacancies requires high local stresses to nucleate a dislocation, resulting in necking, the role of vacancies is to promote a more uniform distribution of strain. It is likely that the presence of extended defects, such as dislocations, produce much stronger effects, eliminating the drop at more realistic concentrations than in the case of vacancies. A video included in the Supplementary Material[31] that shows the deformation of nanowires with and without vacancies, illustrates these comments in a more precise way.

IV. CONCLUDING REMARKS

To summarize, the yield point of aluminum nanowires subjected to uniaxial stretching has been investigated my means of molecular dynamics. The work was mainly focused on the stress drop at the yield point found by different authors and observed experimentally. Calculations were carried out on wires with aspect ratio and average coordination varying in the ranges 0.25–2.35 and 7.9–11.3, respectively. After having checked that neither of those two parameters seem to be essential as far as the occurrence of the drop is concerned, calculations on nanowires containing point defects (vacancies in particular) were carried out. Vacancies reduce both the yield stress and the stress drop. Extended defects, such as dislocations, might produce much stronger effects eliminating the drop at more realistic concentrations than in the case of vacancies. However, as no extended defects are expected to exist in very small nanowires, a drop should exist, as confirmed experimentally. As the size of the wire increases, dislocations will appear reducing gradually the stress drop at the yield point discussed in this work.

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