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Role of temperature in the formation and growth of gold monoatomic chains: A molecular dynamics study

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The effect of temperature on the formation and growth of monoatomic chains is investigated by extensive molecular dynamics simulations using a semiempirical potential based on the second-moment approximation to the tight-binding Hamiltonian. Gold nanowires, with an aspect ratio of ~ 13 and a cross section of ~ 1 nm², are stretched at a rate of 3 m/s in the range of temperatures 5–600 K with 50 initial configurations per temperature. A detailed study on the probability to form monoatomic chains (MACs) is presented. Two domains are apparent in our simulations: one at $T < 100$ K, where MACs develop from crystalline disorder at the constriction, and the other at $T > 100$ K, where MACs form as a consequence of plastic deformation of the nanowire. Our results show that the average length of the formed MACs maximizes at $T = 150$ K, which is supported by simple energy arguments.

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I. INTRODUCTION

The potential use of nanowires as components of electronic circuits will probably shift a paradigm in the miniaturization and design of microchips.¹ From a more fundamental perspective, gold nanowires have been investigated to understand their intriguing mechanical properties and also to shed light on the interplay between low dimensionality and quantum-mechanical effects (for a review see Refs. 2–4).

Formation and evolution of gold monoatomic chains (MACs) have been extensively investigated in experiments.^{5–10} These studies suggest a strong effect of temperature on the tensile deformation of nanometric structures. In particular, stretching at low temperature ($T \leq 150$ K) is a process dominated by the formation of planar defects, whereas at room temperature the deformation seems plastic and defect free.¹⁰ Nevertheless, long, stable MACs form at low temperature⁸ and, perhaps more puzzling,¹¹ at room temperature.⁹

From the computational point of view, the size of the system limits computational investigations aiming at describing stretching of nanometric wires. This is the case for *ab initio* methods that have been used to study stability and breaking conditions of idealized MACs, which consist of a few atoms suspended between model electrodes,^{11–16} and also tight-binding molecular dynamics methods^{17,18} intended to study the interplay of electronic and mechanical properties of stretched nanowires.

To overcome this difficulty, classical molecular dynamics (MD) relying on semiempirical potentials has been widely used to simulate stretched nanowires.^{19–26} The versatility of this method allows the study of structural properties of nanowires such as Young's modulus,²⁷ the stability¹⁷ and breaking of MACs,^{3,4,8} temperature-dependent breaking of thick nanowires,²⁸ and, in combination with tight-binding calculations, the thermopower of metal nanocontacts.²⁹ It

is clear that MD is robust and versatile enough to study temperature-dependent formation of planar defects in stretched nanowires and simultaneously formation, evolution, and breaking of MACs.

In this paper we perform extensive MD simulations of stretched nanowires to investigate the effect of temperature on the formation and growth of MACs. Gold nanowires, with a cross section of ~ 1 nm², are simulated in the range of temperatures $T = 5$ –600 K. Due to the fairly large amount of statistics included in this study, the probability to form MACs as a function of temperature is presented. More important, our results suggest that there is an optimal temperature for creation of long MACs.

This paper is organized as follows. The model and the computational method are defined in Sec. II. Section III starts with the description of some generalities of the stretching process (Sec. III A). The dependence of the probability of MAC formation on temperature is shown in Sec. III B, while the relationship between the average length of the formed MACs and temperature is described in Sec. III C. Finally, a summary is given in Sec. IV.

II. THE MODEL AND THE METHOD

Molecular dynamics simulations are performed using an interatomic potential given by the second-moment approximation (SMA) to the tight-binding Hamiltonian.^{30–34} In the SMA, the total energy of a system of N atoms can be written as

$$E = -\zeta \sum_i^N \sqrt{\sum_{j \neq i}^N e^{-2q(r_{ij}/r_0-1)}} + A \sum_i^N \sum_{j \neq i}^N e^{-p(r_{ij}/r_0-1)},$$

where r_{ij} is the interatomic distance between atoms i and j , r_0 is the equilibrium bulk distance, and the parameters A , ζ , p , and q are obtained from bulk properties such as cohesion

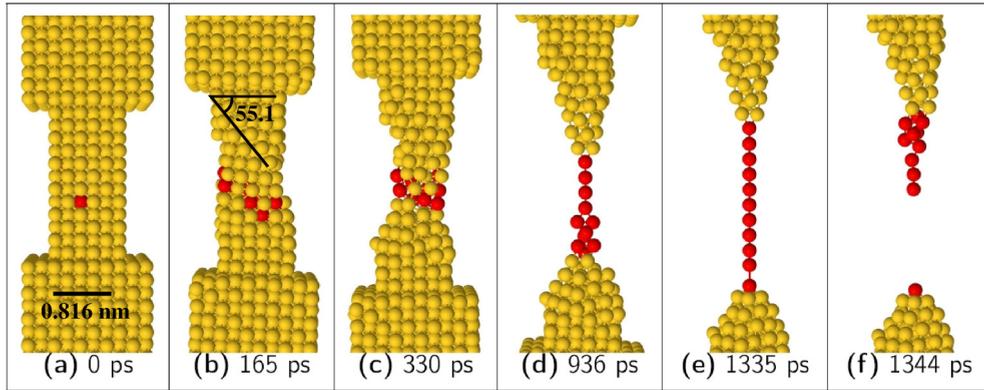
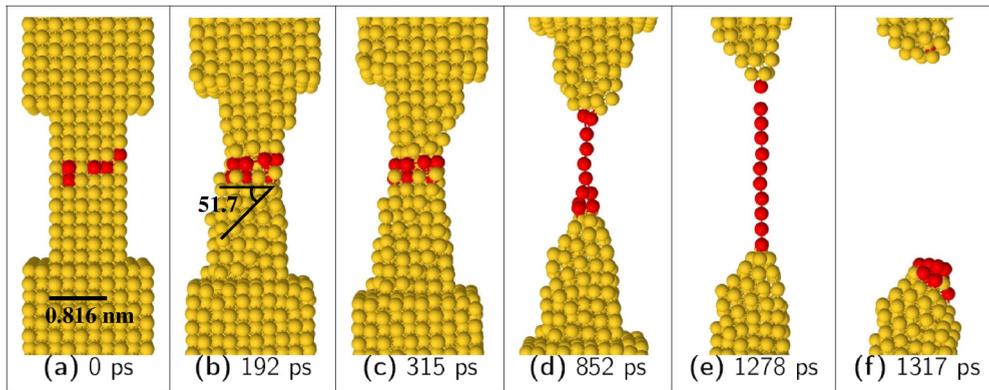
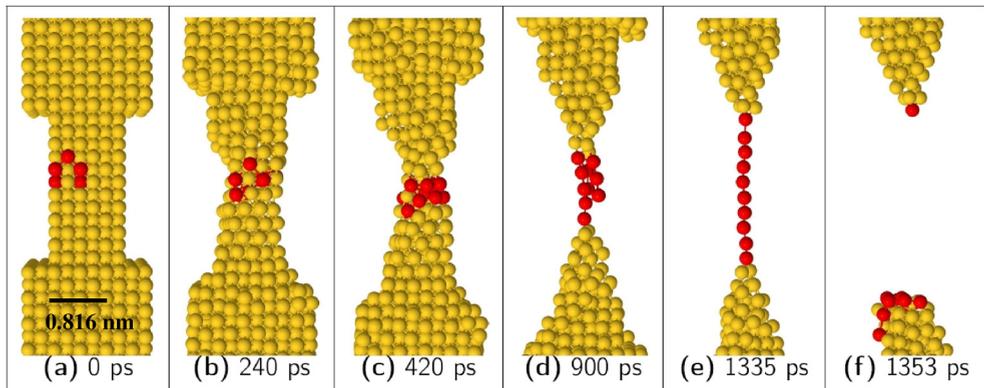
(1) $T=10$ K(2) $T=150$ K(3) $T=300$ K

FIG. 1. (Color online) Snapshots of a stretching sequence for (1) $T = 10$ K, (2) $T = 150$ K, and (3) $T = 300$ K. The wire's cross section is approximately 1 nm^2 , which is comparable to the experimental setup of Ref. 10. The atoms that form the MAC are represented in red (dark gray). The low occurrence probability of these MACs (6%, 2%, and 2% at $T = 10$, 150, and 300 K, respectively) makes them more the exception than the rule.

energy E_c , interatomic distances, and elastic constants. The SMA potential parameters used in our simulations are taken from Ref. 35.

One can expect a limitation of the second-moment approximation for the description of low-coordinated systems due to the fact that parameters for this semiempirical potential are obtained from bulk properties. However, as pointed out by Pu *et al.*,³⁶ SMA potentials give the best results when comparing to DFT energy calculations for the description of structural and mechanical properties of stretched gold nanowires.

In addition, SMA potentials predict a breaking force for gold monoatomic chains in fairly good agreement with experiments.⁸

The systems simulated each contained 1216 atoms arranged in a prismatic fcc structure (see Fig. 1 at 0 ps). This structure was stretched³⁷ along the z direction ([100] direction) until breaking. Previous computational studies²¹ suggest that this direction of elongation favors the formation of long MACs. Periodic boundary conditions were imposed only along the stretching direction, i.e., the z axis.

A MD approach with additional degrees of freedom for the simulation cell was implemented to study systems where volume and shape transformations occur.^{38,39} The atomic positions $\{\mathbf{r}_i\}$ are written in terms of a time-dependent matrix $\mathbf{H}(t)$ and reduced coordinates s_i .

$$\mathbf{r}_i = \mathbf{H}\mathbf{s}_i, \quad \dot{\mathbf{r}}_i = \dot{\mathbf{H}}\mathbf{s}_i + \mathbf{H}\dot{\mathbf{s}}_i,$$

where the dot represents a time derivative. To introduce stretch, only one component of the matrix \mathbf{H} , i.e., H_{33} , evolves in time. In this study, $H_{33} \equiv L_z(t)$, where $L_z(t) = L_z(0) + v_{st}t$ is the total length of the wire at time t and v_{st} is the stretching velocity, which is set to 3 m/s. This value is orders of magnitude larger than experimental ones because it is impossible to reach values of 10^{-7} m/s using current state-of-the-art computing facilities. However, this discrepancy does not prevent this investigation from providing a qualitative picture of temperature effects.

Finally, the equations of motion were integrated using Verlet's algorithm⁴⁰ with a time step of 1 fs, which afforded fairly long simulation times (~ 2000 ps). The temperature of our samples was controlled using the Berendsen thermostat.⁴¹ Moreover, 50 initial configurations per temperature were sampled, and each initial state was defined by a Maxwell velocity distribution. For the present study, a range of temperatures between 5 and 600 K was considered.

III. SIMULATION RESULTS

As mentioned in the Introduction, this section starts by presenting three stretching sequences selected to illustrate particular details of the simulation results (Sec. III A). Then, by using all the data for stretching and temperatures, the probability to form MACs is presented (Sec. III B). Finally, Sec. III C details the evidence suggesting that there is an optimal temperature for the formation of long MACs.

A. Generalities of the stretching process

In Fig. 1 three stretching sequences, from 0 to ~ 1300 ps, at (1) $T = 10$, (2) 150, and (3) 300 K are shown (see Supplemental Material, movies 1, 2, and 3).⁴² These cases were selected because they form long, stable MACs and illustrate particular details of the stretching process. Atoms forming the MAC are red (dark gray) at all times.

Planar defects can be identified at 10 K (165 ps) and 150 K (192 ps). These defects correspond to the well-known fcc slip system with [110]-type directions within (111) planes.⁴³ The angle between (111) and (100) planes is 55.10° at $T = 10$ K and 51.70° at $T = 150$ K, which are close to the ideal 54.75° value expected from geometrical considerations. At room temperature, formation of planar defects is less evident [see Fig. 1, row (3) at 240 ps], and on the few occasions they appear, temperature destroys them rapidly.

These planar defects remain upon stretching at 10 and 150 K, as shown in animations of the system evolution (Fig. 1 at 330 and 315 ps, respectively). By contrast, at room temperature (Fig. 1 at 420 ps), plastic elongation is apparent. This formation of glide planes at low temperature and plastic,

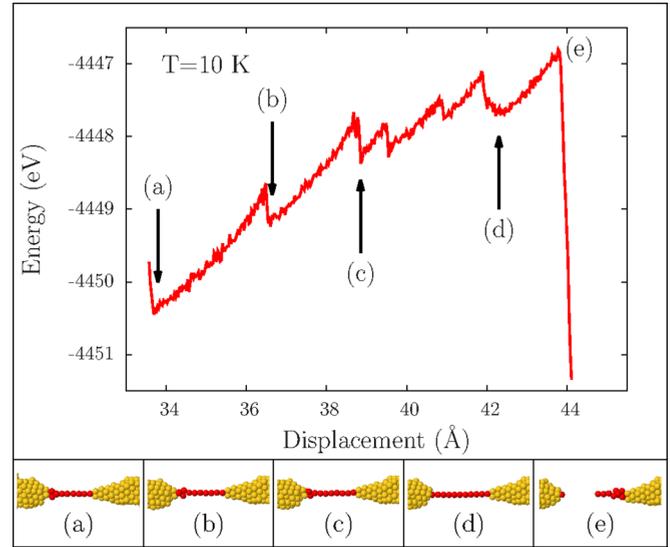


FIG. 2. (Color online) MAC total energy at $T = 10$ K as a function of displacement (\AA). The local minima are related to the addition of an atom to the chain, and the global minimum corresponds to the breaking of the chain.

defect-free stretching at room temperature has been observed experimentally¹⁰ and also discussed in a more general context in Ref. 4.

Our simulations suggest that the growth of MACs also depends on temperature (Fig. 1 around 900 ps). At low temperatures, the contact reduces energy by arranging zigzag chains and dimer-like structures prior to the formation of MACs,^{4,12,21} while at room temperature MACs evolve from bilinear chains.³⁶ Moreover, statistical analysis shows that 80% of the atoms forming the MACs at $T = 300$ K come from the outmost external layers of the nanowire. By contrast, this percentage decreases to almost 50% at $T = 10$ K.

Figure 1 (~ 1300 ps) illustrates the formation of very long MACs (≥ 10 suspended atoms), which have been obtained in the temperature range 10–300 K. Regardless of temperature, MACs grow by taking atoms from one electrode at a time. We observe that the axial symmetry of the electrode limits the size of the MACs.¹⁷ In fact, growth stops only if both contact tips become symmetric (Fig. 1 around 1300 ps) because in this situation to take one atom from the electrode and put it in the chain requires more energy than that liberated from breaking a bond within the chain. Interestingly, the MAC always breaks between the atom closest to one of the two tips and its first neighbor in the chain. This breaking mechanism can be explained by the fact that the atom closest to the contact tip has higher binding energy than the atoms within the MAC, as supported by low-temperature measurements of the effective stiffness of suspended gold chains.^{3,8}

Figure 2 shows a plot of total energy in terms of the elongation of the nanowire at $T = 10$ K. The breaking force of the MAC F_b is evaluated as the slope between points (d) and (e).⁸ We find $F_b = 1.0 \pm 0.2$ nN, in good agreement with previous MD simulations⁸ and slightly lower than the experimental value of 1.5 ± 0.3 nN at 4.2 K.⁸ By evaluating

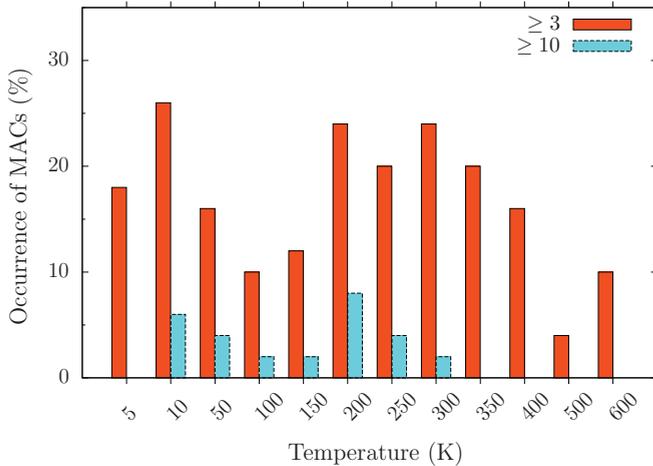


FIG. 3. (Color online) Percentage of formation of MACs as a function of temperature. Red (dark gray) bars show statistics for MACs of more than two atoms; blue (light gray) bars show statistics for MACs of more than nine atoms.

F_b for all the MACs obtained at this temperature, we find that it is independent of the length of the chain, in agreement with experimental results.^{3,8} Moreover, we compute F_b at $T = 5, 10, 50,$ and 100 K. Our results suggest that the breaking force is independent of temperature. To some extent, this result agrees with experimental evidence. Kizuka⁹ has reported $F_b = 1.6 \pm 0.7$ nN at room temperature, which is quite similar to the force measured at 4.2 K.⁸ Once the MAC breaks (last column in Fig. 1), suspended atoms tend to cover the electrode in order to minimize surface energy.⁴⁴

B. Probability to form MACs vs temperature

The probability to form MACs has been evaluated by counting the number of times a chain of three or more suspended atoms is formed. Figure 3 shows a bar diagram with the probability to form MACs as a function of temperature. The probability to form MACs of three or more suspended atoms is around 25% at $T = 10$ K and between $T = 200$ and 300 K. If only very long MACs are considered, i.e., ≥ 10 suspended atoms, the formation probability decreases to $\sim 10\%$. In both cases, the probability distribution has two peaks, one at $T = 10$ K and another around $T = 200$ K.

This particular shape of the probability distribution is interpreted by analyzing the formation of atomic contacts in detail. A magnified view of the nanowire's indented region oriented along the (110) direction is shown in Fig. 4, which displays snapshots of the atomic contact at (1) $T = 10,$ (2) $100,$ and (3) 200 K that correspond to the first maximum, minimum, and second maximum, respectively, in the distribution of Fig. 3. At low temperatures, the gliding induced by stretching produces disorder between crystalline planes. This disorder in the indentation is evident at $T = 10$ K (Fig. 4 at 300 ps). Twisted dimer-like structures (Fig. 4 at 600 ps) and subsequently MACs are formed if atoms at the indentation cannot accommodate symmetrically around the contact tips.

According to the results of Fig. 3, it is less probable to form MACs at $T = 100$ K. The reason is that in most of the cases considered at $T = 100$ K we observe a marked temperature-induced recrystallization of the disordered region, as shown in Fig. 4 at 150, 300, and 450 ps. Formation of highly symmetric contact tips precedes nanowire breaking, as mentioned in the previous section and discussed in detail in Refs. 17 and 14. Therefore, we conclude that temperature-induced recrystallization of the contact tips prevents the formation of MACs.

When temperature increases to $T = 200$ K, the wire reduces its cross section through a plastic deformation process, as can be seen between 150 and 450 ps in Fig. 4. The ductility of the wire has increased with temperature, and as a consequence, the contact tends to form nanorods and double chains (Fig. 4 at 600 ps) that eventually evolve into MACs.

The maximum recrystallization temperature ($T = 100$ K) is related to the interplay of stretching and the rms speed of the atoms. This implies that if the stretching velocity decreases, then the temperature of maximum recrystallization decreases as well, or, in other words, atoms have more time to accommodate if the stretching velocity decreases. This experiment has been performed by reducing the stretching velocity to 1 m/s using smaller nanowires and fewer repetitions of the stretching process, and we observed this dependence of recrystallization temperature and stretching velocity.⁴⁵ Nevertheless, extrapolating to the experimental case (stretching velocity of $\sim 10^{-7}$ m/s), we expect that temperature-induced recrystallization appears at very low temperatures. We therefore expect that further experiments exploring the probability to form MACs with temperature will observe a single-peaked probability distribution and the minimum observed at $T = 100$ K is nothing but an artifact of MD simulations.

C. MAC average length vs temperature

In this section, we focus our attention on the cases where MACs are formed. Energy models have been successfully tested in the past to describe stability and growth of MACs. Thiess *et al.* give a thorough account in Ref. 46. Let us consider a MAC of length L with N suspended atoms. The binding energy of a single atom in an infinite MAC can be written as $E_{\text{MAC}}(d) = E_{\text{MAC}}(d_0) + E(d)$. Here, $d = L/(N + 1)$, d_0 is the equilibrium distance for atoms within the MAC, and $E(d) > 0$ is defined as the binding energy of this atom relative to $E_{\text{MAC}}(d_0)$. Upon stretching, the energy of the MAC grows as $(N + 1)E(d)$, with $N + 1$ being the number of bonds in the chain.

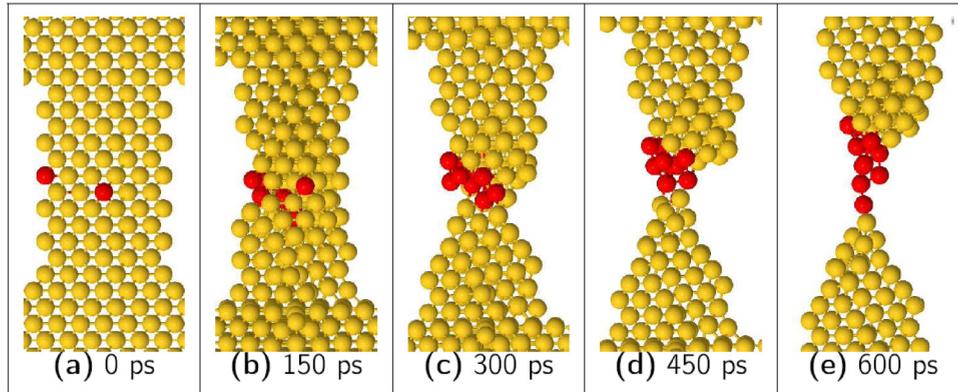
A MAC is stable if the relation

$$NE(d_0) + \Delta E_b \geq (N + 1)E(d)$$

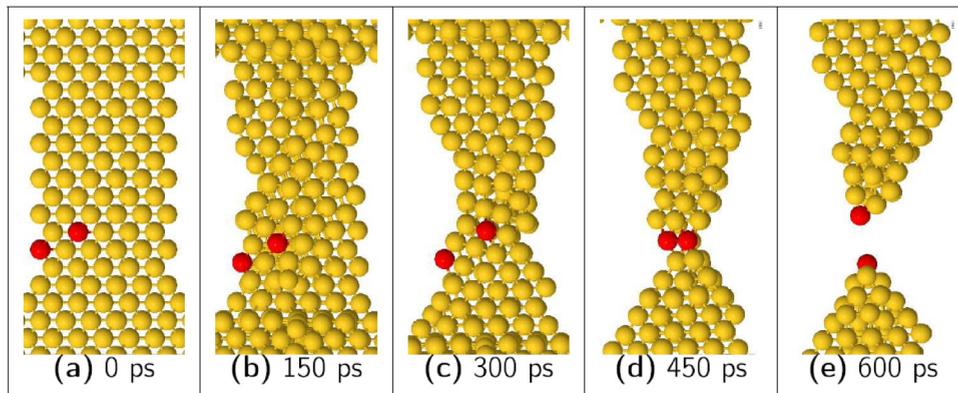
is satisfied. In other words, the MAC is stable if its energy is lower than or equal to the energy of the broken chain $NE(d_0)$ plus the energy necessary to break a bond in the chain ΔE_b . Likewise, a stretched MAC grows if its energy $(N + 1)E(d)$ is greater than the energy of a chain with $(N + 2)$ bonds [and distance between atoms $d' = L/(N + 2) < d$] plus the energy, ΔE_g , necessary to break one bond in the contact tip and create it in the chain, i.e.,

$$(N + 1)E(d) \geq (N + 2)E(d') + \Delta E_g.$$

(1) $T=10$ K



(2) $T=100$ K



(3) $T=200$ K

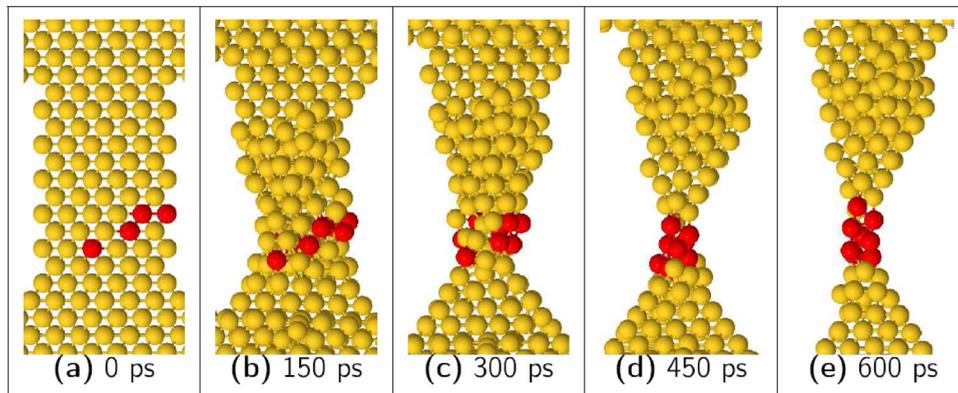


FIG. 4. (Color online) Detail of the formation of the atomic contact at (1) $T = 10$, (2) 100, and (3) 200 K. The central region has been oriented with the [110] direction perpendicular to the paper. The red (dark gray) spheres represent the atoms that form the contact.

Using these two inequalities simultaneously, it can be demonstrated that $\Delta E_b - \Delta E_g = N[E(d') - E(d_0)] + 2E(d') > 0$. $\Delta E_b = 1.5$ eV and $\Delta E_g = 0.5$ eV are estimated values obtained from curves of total energy vs elongation like the one in Fig. 2.

The fact that $\Delta E_b > \Delta E_g$ implies the MAC growth and breaking sequence described below. Upon stretching, the MAC energy $(N + 1)E(d)$ increases since the separation between atoms d increases. If the MAC is stable, eventually, the inequality $(N + 1)E(d) - (N + 2)E(d') \geq \Delta E_g$ is satisfied, and an extra atom is added to the chain. This growth

mechanism continues until the energy difference between the stretched and the broken chain is greater than ΔE_b and finally the MAC breaks. This description neglects temperature effects; however, they can be introduced qualitatively in a simple way. By increasing temperature, atoms in the system increase their kinetic energy and break bonds easily. This implies that the gain in kinetic energy first favors the growth of MACs since in this case atoms likely jump from the contact tip to the chain. However, if the temperature increases above a critical value, suspended atoms have more energy available to break bonds in the chain and reach the global energy minimum $NE(d_0)$. Thus

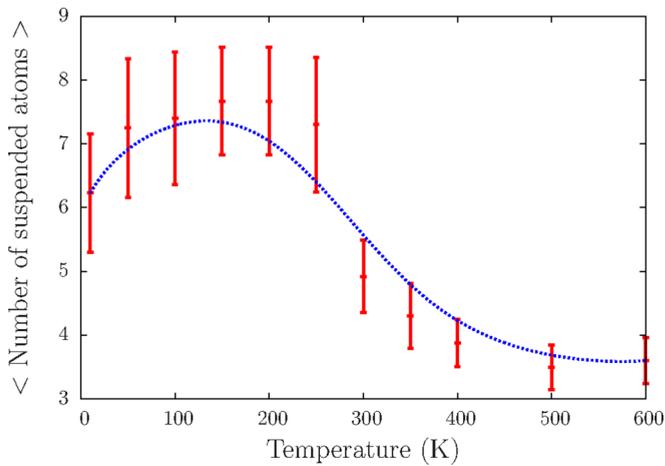


FIG. 5. (Color online) Number of atoms in the MAC as a function of temperature. There is a critical temperature at which the average number of atoms in the chain has a maximum (see text). The dotted blue line is a guide to the eye.

temperatures above the critical value prevent the formation of long MACs. To summarize, by increasing temperature, it is expected that the average number of suspended atoms in the MACs increases as well. Furthermore, if the temperature increases beyond a critical value, then the system prefers to reach the global energy minimum, thus breaking.

To investigate this conjecture, we evaluate the average length of the MACs formed (in terms of the number of suspended atoms in the chain) as a function of temperature (Fig. 5). At very low temperature, $T = 5$ K, the average number of suspended atoms is six. As expected, this number increases when temperature increases until it reaches a maximum of seven to eight suspended atoms at $T = 150$ – 200 K. Above this temperature, the average number of suspended atoms decreases, showing a tendency to break upon increasing temperature.

IV. CONCLUSIONS

We have performed extensive MD simulations of stretched gold nanowires to investigate formation, growth, and breaking of MACs. We have considered nanowires with a cross section of ~ 1 nm² in a range of temperatures ($T = 5$ – 600 K) where it is possible to observe both formation of glide planes and plastic, defect-free stretching. Moreover, we computed the breaking force for MACs formed in the range $T = 5$ – 100 K and found that it is independent of both MAC length and temperature, in fair agreement with experiments.

We found that the probability to form MACs exhibits a double-peaked distribution with maxima at $T = 10$ K and around $T = 200$ – 300 K. The first maximum is related to crystalline disorder at the constriction induced by planar defects at low temperature that favors the formation of MACs. The second maximum is related to the formation of MACs from rodlike structures that appear as a result of plastic deformation. The minimum in the distribution, which has been interpreted as an artifact of MD simulations, has been related to temperature-induced recrystallization at the constriction.

Finally, we found that the average number of suspended atoms in the formed MACs exhibits a maximum at a critical temperature, which in our simulations is about $T = 150$ K. Using a simple energy model, we relate this maximum to the interplay of temperature and the energy necessary to break bonds in the contact tips and within the MAC. This result in particular highlights the importance of temperature in devising models that describe formation, growth, and breaking of MACs.

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