Monte Carlo Simulation Study of Mechanical Properties of Au Nanowires

S. Tanimori* and S. Shimamura**

* VBL, Yamaguchi University, Ube 755-8611, Japan
tanimori@apsci.yamaguchi-u.ac.jp
** Faculty of Engineering, Yamaguchi University, Ube 755-8611, Japan
simamura@po.cc.yamaguchi-u.ac.jp

ABSTRACT

We have carried out Monte Carlo simulations of elongation and shear of Au nanowires to investigate their mechanical properties. We have followed stable atomic arrangements in the nanowires during deformation. The Morse potential has been used as an interatomic interaction. In both elongation and shear, plastic deformation of Au nanowires proceeds in alternating elastic and yielding stages. Force relaxation occurs at each yielding stage. Our simulations predict that Au nanowires break at smaller strains at 600 K than at 300 K in elongation. Young's modulus and the yield stress in elongation estimated from our simulations are in fair agreement with experiments for Au nanowires.

Keywords: Au, nanowire, Monte Carlo simulation, mechanical property

1 INTRODUCTION

The continuing miniaturization of electronic devices has stimulated an interest in nanometer-scale materials such as nanowires and point contacts. Metallic nanowires have received considerable attention in relation to wiring in nanometer-scale integrated circuits in future [1]–[7]. It is important to understand mechanical properties of metallic nanowires to utilize them in the circuits. We study mechanical properties of Au nanowires by means of Monte Carlo simulations.

2 SIMULATION PROCEDURE

We consider a nanowire cut out from bulk Au, as shown in Fig. 1(a). It consists of five atomic layers perpendicular to the wire axis [001], and is put between the top and bottom layers. Each atomic layer includes 12 or 13 atoms, as shown in Fig. 1(b).

The Morse potential [8] is used as an interatomic potential. The potential parameters have been determined [9] so as to reproduce experimental values of the lattice constant, the bulk modulus and the cohesive energy of bulk Au [10].

We simulate elongation and shear of the nanowire. We follow atomic arrangements during deformation of the wire at constant temperature using the Monte Carlo method [9]. The initial atomic arrangement in the wire is relaxed to a thermal equilibrium arrangement. In elongation, the distance between the top and bottom layers is slightly stretched. After that, the atomic arrangement in the stretched wire is relaxed again to a thermal equilibrium one. Such stretching and relaxation are repeated. In shear, the top layer is displaced in the [110] direction slightly. After that, the atomic arrangement in the nanowire is relaxed to a thermal equilibrium one. Such displacement and relaxation are repeated. Atomic arrangements within the top and bottom layers are fixed; this has not caused any notable effect on the deformation process in our simulations.

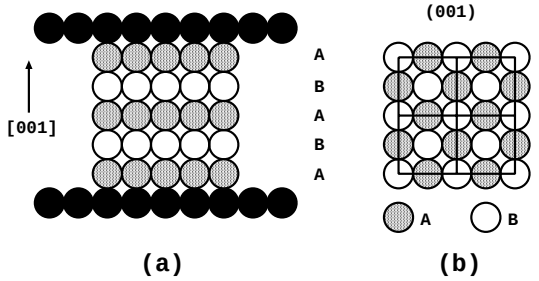

Figure 1: Au nanowire for Monte Carlo simulations: (a) five atomic layers perpendicular to the wire axis [001] are put between the top and bottom layers; (b) atomic arrangement in the cross section of the wire.

We have simulated elongation at 300 K and 600 K, and shear at 300 K.

3 SIMULATION RESULTS

3.1 Elongation

Figure 2 shows the simulation results of the tensile force vs. strain for a Au nanowire at 300 K. The tensile force increases in proportion to strain, and force relaxation (yield) occurs at the strain 0.19. The tensile force again increases linearly with increasing strain and the second yield occurs at the strain 0.43. Thus the elongation of the nanowire proceeds in alternating elastic deformations and force relaxations (yields). After yields occur five times, the nanowire breaks at the strain 0.93. The magnitudes of force relaxation are 3–6 nN except for the first yield. These values are in agreement with

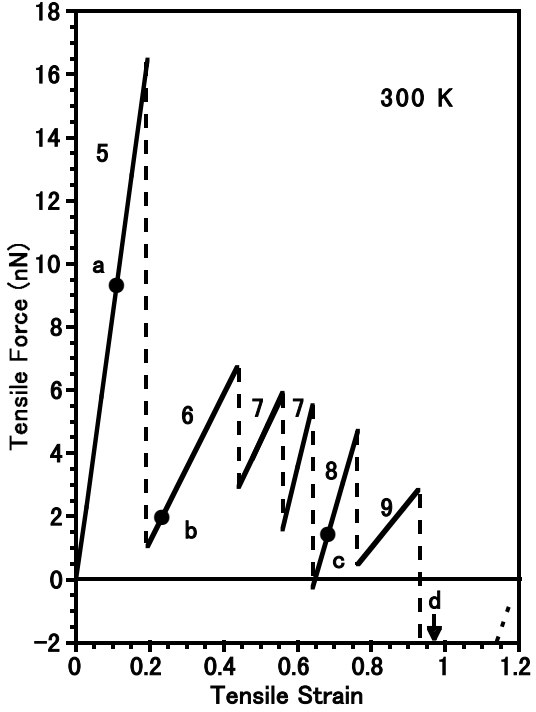

Figure 2: Tensile force vs. strain for a Au nanowire at 300 K. The numerals (5–9) are the number of layers perpendicular to the wire axis. The atomic arrangements at the points **a**–**d** are shown in Figs. 3(a)–3(d), respectively.

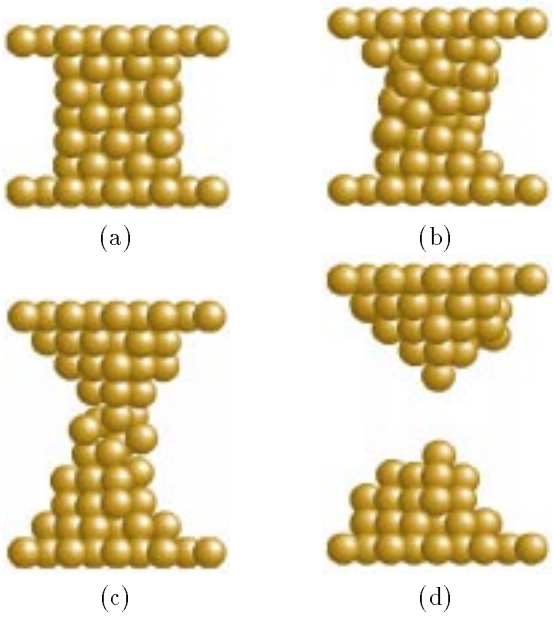

Figure 3: Atomic arrangements in a Au nanowire during elongation at 300 K: (a) at small strain; (b) just after the first yield; (c) after the fourth yield; (d) just after breaking.

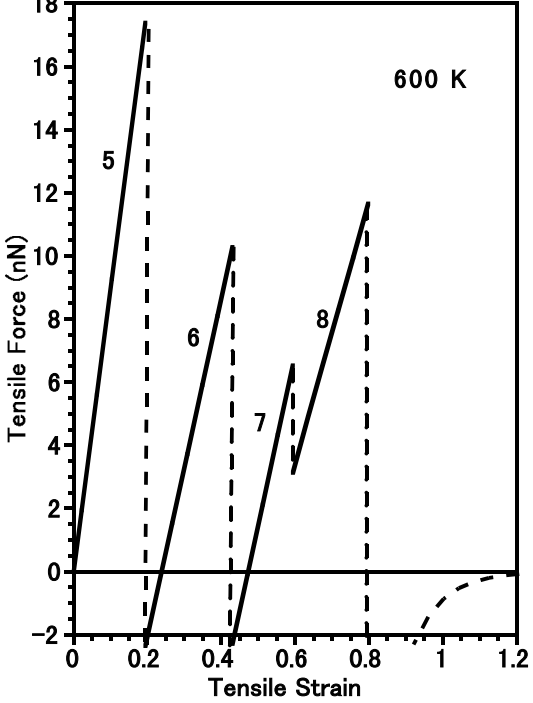

Figure 4: Tensile force vs. strain for a Au nanowire at 600 K. The numerals (5–8) are the number of layers perpendicular to the wire axis.

observed values at room temperature, 2–5 nN [4].

Each force relaxation corresponds to an atomic rearrangement in the nanowire. Figure 3(a) shows the atomic arrangement at the point **a** in Fig. 2. The number of atomic layers is still five except for the top and bottom layers, and the wire elongates uniformly. Figure 3(b) shows the atomic arrangement just after the first yield (the point **b** in Fig. 2). The yield corresponds to an abrupt slipping event on the {111} plane. Several atoms move at a time on the {111} plane. Consequently, the number of atomic layers increases from five to six. At the second yield, the similar slipping event occurs on the {111} plane and the number of atomic layers increases from six to seven. Figure 3(c) shows the atomic arrangement after the fourth yield (the point **c** in Fig. 2). The number of atomic layers is eight. Figure 3(d) shows the atomic arrangement just after breaking (the point **d** denoted by an arrow in Fig. 2). The stretched wire shrinks rapidly so as to release accumulated elastic energy.

Figure 4 shows the simulation results of the tensile force vs. strain for a Au nanowire at 600 K. The elongation of the nanowire also proceeds in alternating elastic deformations and force relaxations (yields). The number of yields at 600 K is less than that at 300 K. The nanowire at 600 K breaks at the smaller strain 0.79 than at 300 K. This is due to thermal motion of atoms acti-

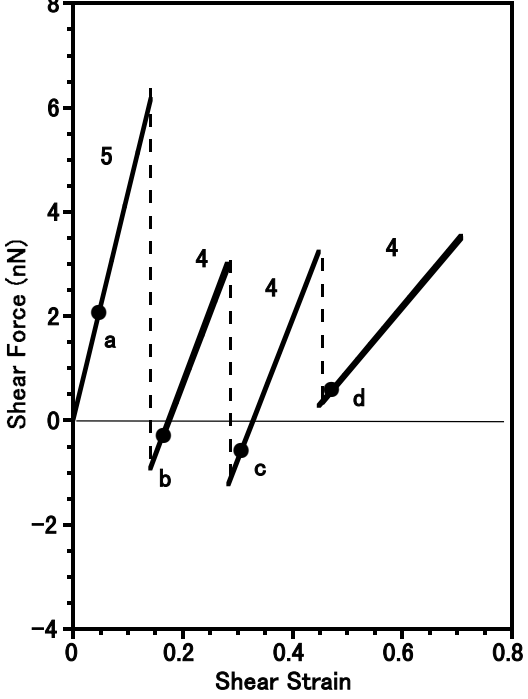

Figure 5: Shear force vs. strain at 300K. The number of layers perpendicular to the wire axis is denoted by the numerals (4 and 5). The atomic arrangements at the points **a**–**d** are shown in Figs. 7(a)–7(d), respectively.

vated in the neck of the wire at high temperatures. The effect of temperature on elongation of Au nanowires has not yet been investigated experimentally. Experimental studies are expected to verify our simulation results.

3.2 Shear

Figures 5 and 6 show the shear force vs. strain for Au nanowires at 300 K. The numerals attached to solid lines denote the number of layers perpendicular to the wire axis. The shear deformation also proceeds in alternating elastic and yielding stages. Our simulations have shown two types of variations in the number of layers. In one type, the number of atomic layers decreases from five to four at the first yield and remains four after that, as shown in Fig. 5. In the other type, the number of atomic layers keeps five during deformation, as shown in Fig. 6.

Figures 7(a)–7(d) show atomic arrangements at the points **a**–**d** in Fig. 5, respectively. As shown in Fig. 7(a), the number of layers is still five at the small strain (the point **a** in Fig. 5), except for the top and bottom layers. The number of layers decreases from five to four just after the first yield (the point **b** in Fig. 5), as shown in Fig. 7(b). The number of layers in Fig. 7(c) also remains four. In Fig. 7(d), a slip occurs on the plane perpendicular to the wire axis, as denoted by an arrow.

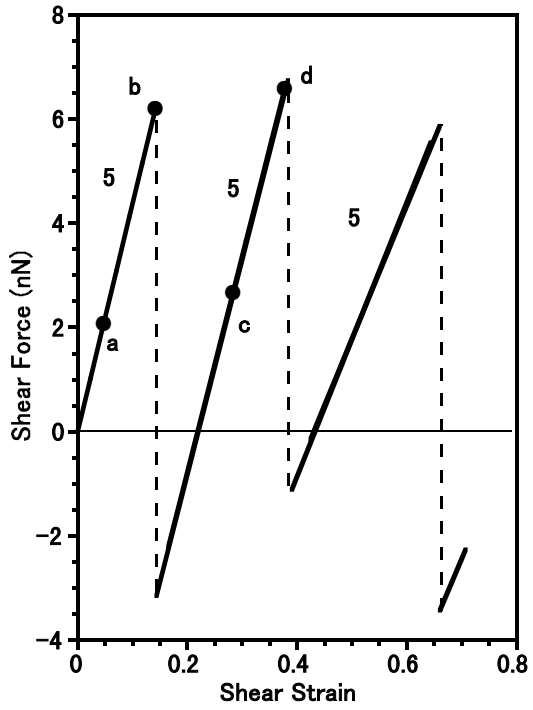

Figure 6: Shear force vs. strain at 300K. The number of layers perpendicular to the wire axis remains five. The atomic arrangements at the points **a**–**d** are shown in Figs. 8(a)–8(d), respectively.

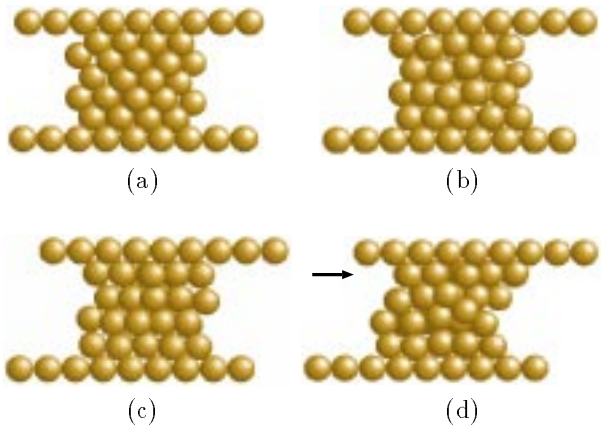

Figure 7: Atomic arrangements in a Au nanowire during shear at 300 K: atomic arrangements (a)–(d) correspond to the points **a**–**d** in Fig. 5. The number of atomic layers decreases from five in (a) to four in (b). The arrow denotes the slipped layer.

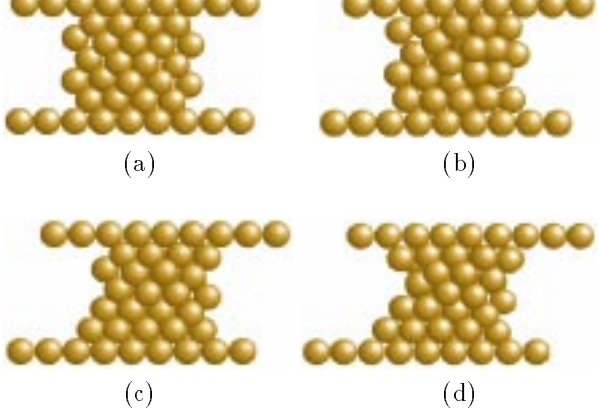

Figure 8: Atomic rearrangements in a Au nanowire during shear at 300K: atomic arrangements (a)–(d) correspond to the points **a**–**d** in Fig. 6. The number of atomic layers remains five.

Atomic arrangements at the points **a**–**d** in Fig. 6 are shown in Figs. 8(a)–8(d), respectively. The number of atomic layers remains five. In Fig. 8(b) corresponding to the point **b** in Fig. 6, we can see a slightly disordered arrangement just before the first yield. However the wire recovers an ordered arrangement after the first yield occurs, as shown in Fig. 8(c).

3.3 Elastic Modulus and Yield Stress

Our simulations have shown that the force of Au nanowires varies in a sawtoothed manner in both elongation and shear. We have estimated Young's modulus E and the shear modulus G from the force-strain relation in small strains. The yield stresses $\sigma_{\rm y}$ in both elongation and shear have also been estimated from the force at the first yield. Table 1 lists the values of these quantities estimated from our simulations, together with experimental values for Au nanowires [4] and bulk Au [11]. The values of E and $\sigma_{\rm y}$ in elongation estimated from our simulations are in fair agreement with experiments for Au nanowires. Young's modulus and the shear modulus of a Au nanowire are the same order of magnitude as large as those of bulk Au. This fact suggests that elastic constants are almost invariant even if the size of a wire becomes nanometer-scale. On the contrary, the yield stress in elongation of a Au nanowire is one order of magnitude larger than that of bulk Au. The yield stress in shear of a Au nanowire is the same order of magnitude as large as the ideal shear strength of bulk Au, 4 GPa. In a dislocation-free nanowire, several atoms slip at a time, as mentioned before. This requires higher yield stresses in a nanowire than in bulk.

Table 1: Elastic modulus and yield stress of Au nanowire (simulation and experiment) and bulk: E, G and $\sigma_{\rm y}$ are Young's modulus, the shear modulus and the yield stress, respectively.

	elongation		shear	
	E/GPa	$\sigma_{\rm y}$/GPa	G/GPa	$\sigma_{\rm y}$/GPa
simulation	80	8	45	6
experiment	40–100	2–8	–	–
bulk	79	0.2	26	–

4 CONCLUSION

We have simulated elongation and shear of Au nanowires using the Monte Carlo method. Plastic deformation proceeds in alternating elastic and yielding stages both in elongation and in shear. In each yielding stage, force relaxation occurs. Elastic constants in nanowires are the same order of magnitude as large as those in bulk. The yield stresses in nanowires are much larger than those in bulk.

ACKNOWLEDGMENT

This work was supported by grants from the Electric Technology Research Foundation of Chugoku and the UBE Foundation.

REFERENCES

[1] J. I. Pascual, J. Méndez, J. Gómez-Herrero, A. M. Baró, N. Garcia, Uzi Landman, W. D. Luedtke, E. N. Bogachek and H.-P. Cheng, Science, **267**, 1793, 1995.

[2] L. Olesen, E. Lægsgaard, I. Stensgaard, F. Besenbacher, J. Schiøtz, P. Stoltze, K. W. Jacobsen and J. K. Nørskov, Phys. Rev. Lett., **72**, 2251, 1994.

[3] N. Agraït, G. Rubio and S. Vieira, Phys. Rev. Lett., **74**, 3995, 1995.

[4] G. Rubio, N. Agraït and S. Vieira, Phys. Rev. Lett. **76**, 2302, 1996.

[5] Uzi Landman, W. D. Luedtke, N. A. Burnham and R. J. Colton, Science, **248**, 454, 1990.

[6] T. N. Todorov and A. P. Sutton, Phys. Rev. B, **54**, R14234, 1996.

[7] M. R. Sørensen, M. Brandbyge, and K. W. Jacobsen, Phys. Rev. B, **57**, 3283, 1998.

[8] L. A. Girifalco and V. G. Weizer, Phys. Rev. **114**, 687,1959.

[9] S. Tanimori, K. Ishida, O. Sueoka and S. Shimamura, J. Phys. Soc. Jpn. **68**, 3556, 1999.

[10] C. Kittel, "Introduction to Solid State Physics" 7th. ed., John Wiley & Sons, Inc., p.23, p.57, p.59, 1996.

[11] *Smithells Metals Reference Book*, 7th ed., ed. E. A. Brandes and G. B. Brook Butterworth–Heinemann Ltd. Chap.15, p.2, Chap.22, p.159, 1992.