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Determination of Temperature-Dependent Elasto-Plastic Properties of Thin-Film by MD Nanoindentation Simulations and an Inverse GA/FEM Computational Scheme

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Abstract: This study presents a novel numerical method for extracting the temperature-dependent mechanical properties of the gold and aluminum thin-films. In the proposed approach, molecular dynamics (MD) simulations are performed to establish the load-displacement response of the thin substrate nanoindented at temperatures ranging from 300–900 K. A simple but effective procedure involving genetic algorithm (GA) and finite element method (FEM) is implemented to extract the material constants of the gold and aluminum substrates. The material constants are then used to construct the corresponding stress-strain curve, from which the elastic modulus, yield stress and the tangent modulus of the thin film are subsequently derived. Results from high-temperature (900 K) nanoindentation MD simulation show that the value of elastic modulus of the gold and aluminum thin-films could decrease by 63.9% and 73.1%, respectively, as compared with the room temperature values. The resulting temperature-dependent stress-strain curves presented in this paper provide the crucial requirement for quantitative computer simulation of nanofabrication process.

Keywords: Thin film, Temperature-dependent mechanical properties, Molecular dynamics (MD), Genetic algorithm (GA), Finite element method (FEM).

1 Introduction

Metal thin films and coatings with thicknesses as little as several nanometers are widely applied in a variety of applications nowadays, including micro-electro-mechanical systems (MEMS), nano-electro-mechanical systems (NEMS), interconnection of electronic packaging systems, optical films, and so forth. Many of

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the thin film applications, however, may experience elevated temperatures. For effective designing and accurate evaluation of the structure integrity, quantitatively characterizing the thermal mechanical properties of the metal thin film is increasingly demanded for the applications. Nanoindentation is the most frequently used technique for measuring thin film properties such as elastic modulus and hardness [Oliver and Pharr (1992)]. In the nanoindentation method, the mechanical properties of the thin film are determined by converting the force-displacement curves generated during the loading and unloading steps into a corresponding material properties. However, obtaining meaningful experimental results becomes increasingly difficult as the characteristic size of the thin film reduces due to the relatively greater effect of equipment limitations such as the machine resolution, the tip-rounding effect, the signal-to-noise ratio of the detection system, and so on. Moreover, environmental factors such as the ambient temperature and humidity have a significant effect on the mechanical properties of typical thin-film materials, but are difficult to quantify experimentally. Accordingly, various researchers have enhanced the original nanoindentation test procedure to improve the reliability of its results [Jayaraman, Hahn, Oliver, Rubin and Bastias (1998); Bouzakis and Vidakis (1999); Pelletier, Krier, Cornet and Mille (2000); Qian, Cao, Zhang, Raabe, Yao and Fei (2008)]. Other researchers have employed finite element method (FEM) techniques to optimize the nanoindentation experimental procedure or to support the evaluation of the nanoindentation test results. For example, Pelletier, Krier, Cornet and Mille (2000) assumed the thin-film material to be characterized by a bilinear stress-strain relationship and employed FEM simulations to determine the optimal tip radius of the indenter. Although the FEM schemes presented in the literature enable the plastic behavior of the thin film to be inversely extracted from the experimental load-displacement curve, they assume the nanoindentation test to be performed at room temperature. However, as discussed above, the mechanical properties of thin-film systems are highly sensitive to the temperature conditions, and thus some form of technique is required to account for both the indenter-to-film interactions and the temperature dependency of the mechanical properties of the indented film.

Molecular dynamics (MD) simulations provide a powerful technique for measuring the materials strength and evaluating the temperature dependency of the physical quantities of interest in nanoindentation tests [Li and Yip (2002); Liang, Woo, Huang, Ngan and Yu (2004); Nair, Farkas and Kriz (2008)]. Hsieh, Ju, Li and Hwang (2004) performed a series of simulations at temperatures ranging from 300–1300 K to analyze the correlation between the system temperature and the nanoindentation results and to identify the critical temperature for the transition of plastic flow mechanism in the copper substrate. Utilizing a three-dimensional MD model, Liu, Fang and Lin (2007) showed that elastic modulus for the gold films were approximately 110–130 GPa obtained from experiment at room temperature, while it was 78–129 GPa for the MD analysis. The authors suggested that the difference between the two sets of results could be attributed to scale differences and the simulation's assumption of a perfect defect-free monocrystalline gold, whereas the experimental workpieces may contain a variety of defects.

In this paper, we consider a similar approach to the author's previous work [Liu and Tsai (2009)], and apply the systematic method of genetic algorithms (GAs) instead of an artificial neural network (ANN) to obtain the material properties of gold and aluminum thin films. The use of ANN is appropriate for predicting the materials parameters with a simple constitutive model, and the method only needs few FE simulations to construct the training data [Husain, Guniganti, Sehgal and Pandey (2009)]. However, as the indented material was modeled using a complicated material model, it is difficult to define a proper parameter domain to train an ANN and the initial training data chosen could highly affect the result prediction from ANN. Moreover, it is difficult to add in additional constrains between the data evaluated from ANN. The current study presents a numerical method comprising MD simulations, a FE model and a GA to extract the temperature-dependent mechanical properties of the thin monocrystalline gold and aluminum substrates. In the proposed approach, MD simulations are performed to establish the load-displacement curves corresponding to nanoindentation tests performed at temperatures ranging from 300–900 K. Utilizing the MD simulation results to define elastic modulus of the thin film; the coupling between the FE simulations and the GA developed are then used to search through a large number of possible material constants (yield stress and tangent modulus) to discover the best specific solution that minimizes the difference of load-depth curve between MD and FEM results. The corresponding values of the material constants are found until satisfactory convergence is achieved. Finally, the predicted values of these constants are used to construct the corresponding stress-strain curve, from which the elastic modulus, yield stress and tangent modulus of the indented gold and aluminum substrates are then obtained. The flowchart diagram of the developed numerical method described above to determine the temperature-dependent mechanical properties of a thin film is demonstrated in Figure 1. The validity of the inversely-derived stress-strain curves can be confirmed by using the associated stress-strain data to recreate the corresponding FE load-displacement curves and then comparing these curves with those obtained from the MD simulations.

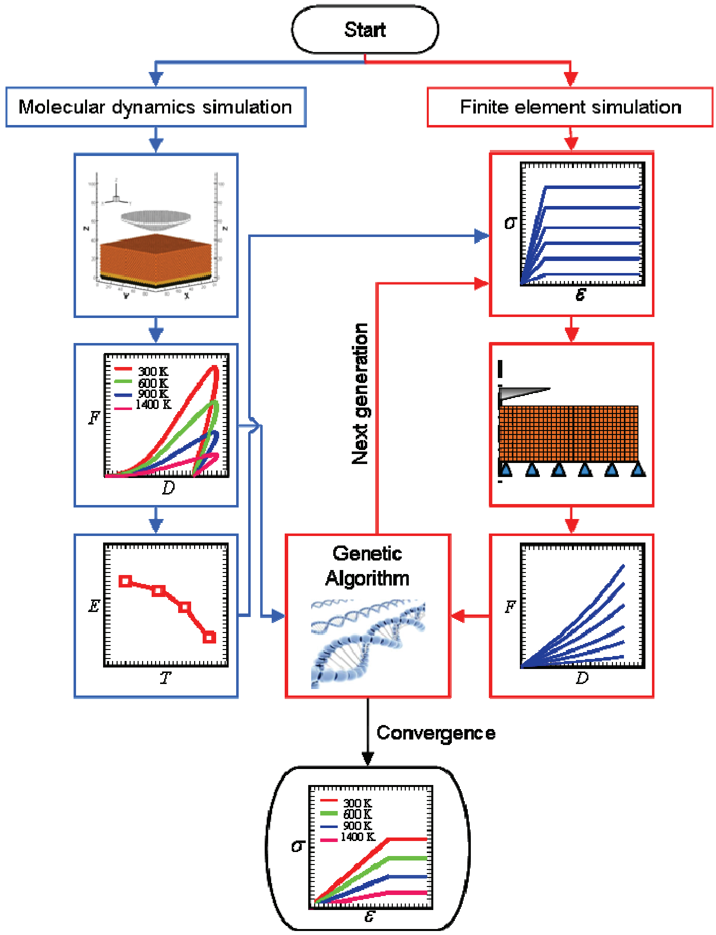


Figure 1: Flowchart diagram to determine a thin film temperature-dependent elastic-plastic stress strain curves, based on the FEM/GA and MD evaluation of nanoindentation results.

2 Molecular dynamics simulation

The MD simulations applied in this paper have been used to investigate the phenomena occurring during the nanoindentation process in author's previous studies [Liu and Tsai (2009)]. Similar method was used to model the nanoindentation of gold and aluminum substrates with face-centered cubic (fcc) structure using either a rigid diamond tip or a conical indenter. Figure 2 presents a schematic illustration of the corresponding MD model. The indented substrate consists of 40 layers of atoms with 1250 atoms in each layer, giving a total of 50000 atoms and the tip radius of the indenter was specified as 10 Å, while the half-angle was assigned a value of 60°. The periodic boundary conditions were imposed in the x- and y-directions, and the lower two layers form a fixed boundary which prevents the substrate from moving in the z-direction during the indentation process.

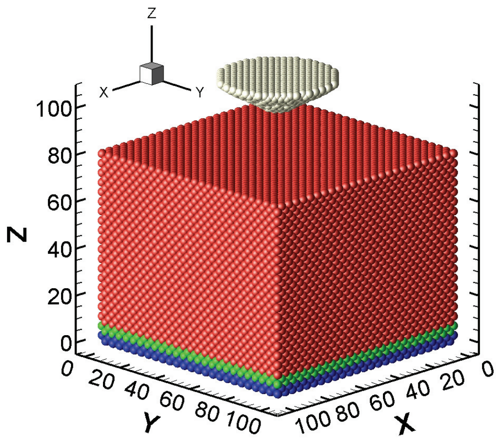


Figure 2: MD model used in nanoindentation tests.

In the simulations, the time step was specified as $\Delta t = 1$ fs, and the positions and velocities of the atoms in the indenter and substrate at each time step were computed from the corresponding data in the previous step using the Gear's fifth-order predictor-corrector method [Haile (1992)]. The interactions between the atoms in the substrate were modeled using the Tight-Binding potential function, i.e.

$$E = \sum_{i=1}^{N} \left\{ Ae^{-p\left(r_{ij}/r_0-1\right)} - \left[\sum_{j} \xi^2 e^{-2q\left(r_{ij}/r_0-1\right)} \right]^{1/2} \right\}, \tag{1}$$

where r_{ij} is the distance between atoms i and j, r_0 is the first-neighbor distance in the fcc lattice, and the constants A, ξ, p and q employed in the simulations are shown in Tab 1 [Cleri and Rosato (1993)].

The interactions between the atoms in the substrate and the carbon atoms in the indenter were modeled using the Morse potential, i.e.

$$\phi(r) = D\left(e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right), \tag{2}$$

Table 1: Parameters used in Tight-Binding potential for indented materials

	$A\,(eV)$	$\xi\,(eV)$	p	q
Au	0.2061	1.790	10.229	4.036
Al	0.1221	1.316	8.612	2.516

where r is the length of the gold-carbon bond or aluminum-carbon bond and D, α and r_0 denote the cohesive energy, the elastic modulus, and the atomistic distance under equilibrium conditions, respectively. The values assigned to D, α and r_0 in the present simulations are summarized in Table 2.

Table 2: Parameters used in Morse potential for tip and substrates

	$D\,(eV)$	$\alpha\left(10^{10}m^{-1}\right)$	$r_0\left(10^{-10}m\right)$
Au-C	1.4915	2.0960	2.7220
Al-C	1.3466	2.1025	2.8875

In MD simulation, the initial velocities of atom are assigned from the Maxwell distribution, and the magnitudes are adjusted by rescaling method [Haile (1992)] so as to keep the temperature in the system constant to according to the following equation:

$$V_i^{new} = \left\{ 3Nk_bT \left[\sum_{j=1}^{N} m \left(V_j^{old} \right)^2 \right]^{-1} \right\}^{1/2} \times V_i^{old}, \tag{3}$$

where V_i is the velocity of atom i, T is a specified temperature, k_B is Boltzmann's constant (1.38×10^{-23} JK^{-1}), m is mass of atom and N is the freedom of the system. The simulations were performed to investigate the effect of the system temperature on the temperature-dependent mechanical properties of the thin film materials at temperatures ranging from 300–900 K. Prior to each simulation, the indenter was positioned at a height of 10 Å above the substrate surface and was then moved through a vertical distance of 18 Å at a rate of 50 m/s. Having reached the indenter at the position of maximum load, it was returned to its original position at the same speed.

3 Overview of genetic algorithms

Genetic algorithm (GA) is used to search through a large number of possible solutions to discover the best specific solution. It is a problem-solving technique that attempts to evolve solutions in a stochastic (or random search) manner much as nature does. Its power lies in that it strikes a reasonable balance between two conflicting search objectives: exploiting the best solutions currently available, and robustly exploring the space for a new solution. Much of the original work on GA was performed by Holland (1975), the working scheme for the GA can be described in brief as follows:

- The GA uses an encoding of parameters instead of the parameter values;
- The GA works on a population of points not on a single point;
- The GA uses probabilistic rules to obtain a satisfying result according to the natural law of evolution;
- The GA uses simple operations on the objective function value, no complex calculations such as derivation are necessary;
- The GA involves a set of genetic operators: selection, crossover and mutation.

In the GA optimization process, once the initial population is randomly created, the rules must be defined according to the point that would have the potential to evolve with a high probability towards the desired global optimum. The first genetic operator is selection (or called reproduction). The principle of the GA is that the best points in the population, i.e. the closest to the optimum, must have a greater chance for survival and reproduction than the worst points in the population. This is the purpose of the selection operator. Several types of selection operators have been described by De Jong (1975). The most popular one is the proportional selection operator, also called "roulette wheel selection". The selection operator determines members of the population to participate in the production of members for the next population. Selection is based upon the value of the fitness function or the fitness of individual members, such that members with greater fitness levels tend to survive. Crossover recombines the traits of the selected members, in the hope of producing an offspring with a better fitness level than its parents. Crossover sites are defined for each pair by generating random numbers for exchanging data between the parents. After crossover, the next process is mutation. The principle of mutation was developed by Foo and Bosworth (1972). It consists of the modification of one gene (i.e. one bit of the string). A probability for mutation is given for each element in the population. If a randomly selected number of individuals is superior to a fixed threshold, one bit in each individual is chosen at random and its value is changed from 0 to 1 or 1 to 0. The GA exhibits superior efficiency in global searches compared to the traditional optimization methods. It is able to explore a wide range of potential solutions with lower computational effort based on natural selection, mating and simulation. These advantages demonstrate that the GA is applicable to all kinds of engineering applications [Amaziane, Naji and Ouazar (2004); Amaziane, Naji, Ouazar and Cheng (2005)].

4 Inversely analysis procedure

The objective of the MD simulations described above is to determine the resultant force acting on the indenter tip at each value of the tip displacement in order to construct the corresponding load-displacement curve under each of the considered testing temperatures. The load data are then applied to the developed FEM/GA computational method in order to inversely derive the corresponding stress-strain curve such that the mechanical properties of the thin film can be extracted. In the present study, a FE analysis of the nanoindentation process is constructed using the ABAQUS FE solver and a GA is then employed to optimize the material constants such that the load-displacement curve produced by FE simulation is approximately equal to the MD result. The GA optimization procedure applies the mean square error (MSE) of load data as the objective function:

$$OF = \sqrt{\sum_{i=1}^{N} (F_{MD} - F_{FEM})^2} \tag{4}$$

where
OF: Objective function
i: Number of discretizing point
N: Total number of discretizing point
F_{MD}: Force data from MD simulation
F_{FEM}: Force data from FEM simulation

Note that the force data (F_{MD} and F_{FEM}) represent the reaction force acting on the indenter during the indentation process, which are obtained initially by discretizing the load-displacement curve obtained in the MD and FE simulation using a uniform displacement interval.

Figure 3 presents a schematic illustration of the 2-D axisymmetric FE model constructed using the ABAQUS FE solver. Note that in the FE simulations, the nodes at the base of the model were prevented from moving in the x- or y-directions, while the nodes along the axisymmetric axis were constrained in the x-direction. As in the MD simulations, the FE analysis considers a conical indenter with a tip radius of 10 Å and a half-angle of 60°. The thickness of the film is equal to the MD model. The FEM analysis simulated the indentation process over both the loading and the unloading stages similar as MD simulation. During the loading process, the indenter was pushed into the substrate using a displacement control mechanism and the changing depth is monitored. For a given displacement, the corresponding load at each incremental depth was computed from the reaction force acting on the indenter. The friction between the indenter and the substrate has a negligible effect on the nanoindentation analysis [Pelletier, Krier, Cornet and Mille (2000)], and it was assumed to be frictionless in the FE simulation. The gold and aluminum films were assumed to experience an incremental plasticity effect with isotropic hardening during the indentation process, and its behavior was modeled using the following constitutive equation:

$$\sigma = E\varepsilon, \text{ for } \varepsilon \leq S_y/E$$

$$\sigma = E_t\varepsilon + (1 - E_t/E)S_y, \text{ for } \varepsilon > S_y/E \tag{5}$$

where E, S_y and E_t are material constants and σ and ε are the stress and strain, respectively. Note that the elastic modulus E can be obtained from the results of MD nanoindentation simulation.

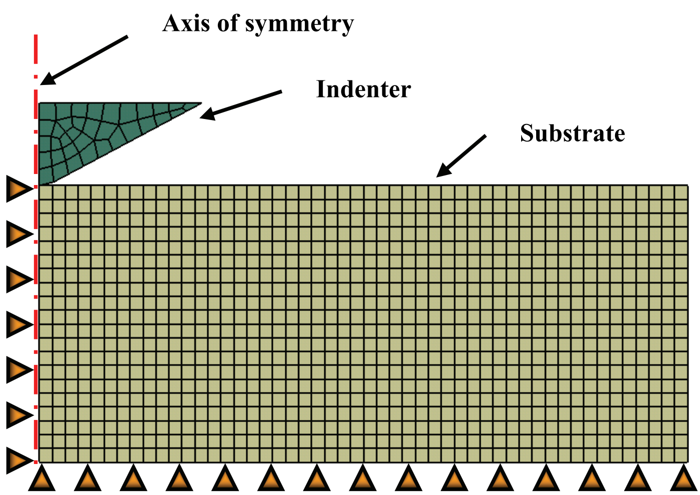


Figure 3: Finite element mesh used to model indentation process. (Note corresponding boundary conditions are also shown).

The GA (in conjunction with the FE model) was then used to determine the optimal value of each parameter by following steps:

1. Initial population of individual material parameters S_y and E_t are constructed randomly within the range 10–5000 MPa and 0–500 MPa. The size of initial population is selected as 20, that means, for each generation 20 FE simulations need to be performed.

2. Each design parameter can be encoded as a L-bit binary number by

$$2^L = \frac{D_{\max} - D_{\min}}{\delta} + 1 \tag{6}$$

where Dmax and Dmin are the upper and lower bounds for the parameter, δ is the coefficient to increase the digit of precision. The binary codes for all design parameters are converted into a sequence binary string.

3. For each individual population, using FE simulation to perform indentation testing simulation under indented depth 8 Å; the data of load-displacement curves are obtained.

4. Using Eq. (4), the fitness value and fitness factor for each individual are calculated.

5. The individuals are coupled randomly and the reproduction operator is applied. Using two points crossover with probability 0.80, the new population is obtained.

6. Mutation is applied to the new population with a probability value of 0.001 as suggested in [Chen and Chen (1997)].

7. The initial population is replaced by the new population and steps 1-6 are repeated till a pre-assigned number of generations are reached. After a number of trials with different generations, it is found that after 50 generations there is no significant change in all material parameters.

8. The genetic parameters and schemes used in the optimization procedure are summarized in Table 3.

In GAs the processes of selection, crossover, and mutation are repeated until satisfactory convergence is achieved and the optimum solution (material constants S_y and E_t) is found. These material constants are used to construct the stress-strain curve, from which the yield stress and tangent modulus of the indented material are then derived. Finally, the inversely-derived stress-strain curves of gold and aluminum films are obtained

Table 3: Genetic parameters and schemes used in GA optimization procedure

Number of generations	50
Number of populations	20
Encoding scheme	Float binary precision encoding
Selection scheme	Ranking selection based on the normalized geometric distribution
Crossover scheme	Two points crossover
Mutation scheme	Non-uniform probability distribution changes one of the parameters of the parent
Rank selection probability	0.08
Crossover probability	0.80
Mutation probability	0.001

5 MD simulation results

The MD nanoindentation simulations were performed using the gold and aluminum substrates and a diamond conical indenter at temperatures of 300 K, 600 K and 900 K, respectively. Note that in the simulations, the load acting on the diamond indenter was obtained by summing the resultant forces contributed by the surrounding substrate atoms in the z-direction. The corresponding load-displacement curves are presented in Figure 4 and Figure 5; and deformed shape after indentation at the temperature of 300 K is illustrated in Figure 6. Overall, the results show that for a given indentation depth, the applied load decreases as the temperature increases. In other words, the substrate material exhibits a softening effect at high temperatures. Utilizing these load-displacement curves, the elastic modulus of the gold and aluminum films at each of the test temperatures was estimated using the method presented by Oliver and Pharr (1992). The results presented in Figure 7 show that the elastic modulus of the gold substrate varies from 123–44 GPa over the temperature range of 300–900 K, and the elastic modulus of aluminum films is found to be 80–21 GPa, respectively. The present MD analysis results for gold film compare to an elastic modulus range of 110–130 GPa obtained from experiment at room temperature range in [Liu, Fang and Lin (2007)]. It can be seen that reasonable results are obtained from the MD simulation.

6 Inversely analysis results

As described earlier, the coupling between the FE simulations and the GA developed in this study is used to search through a large number of possible material

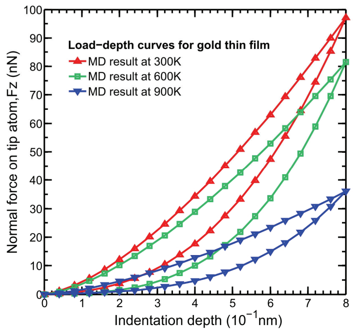


Figure 4: MD simulation results of the load-displacement curves of the thin gold film at temperatures ranging from 300–900 K.

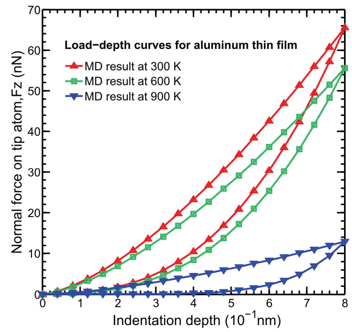
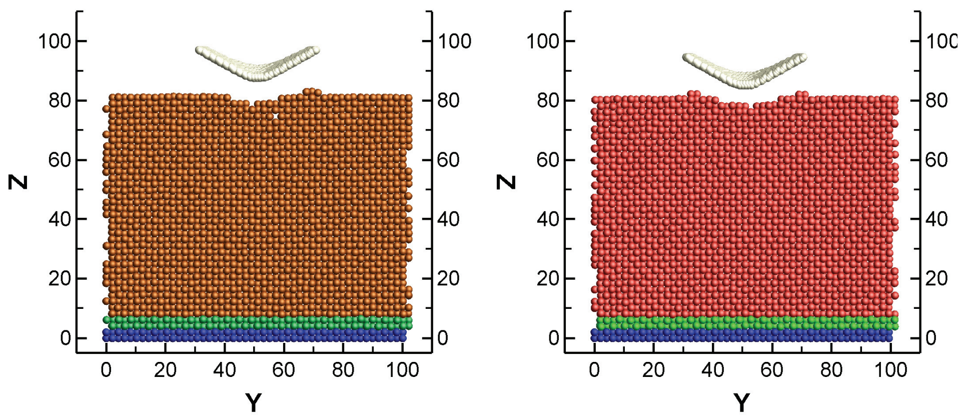


Figure 5: MD simulation results of the load-displacement curves of the thin aluminum film at temperatures ranging from 300–900 K.



(a) (b)

Figure 6: Atomic configuration of (a) gold and (b) aluminum substrates after nanoindentation at temperature 300 K.

constants (yield stress and tangent modulus) to discover the best specific solution that minimizes the mean square error of the load-depth curve between the MD and FEM results. By substituting the typical elastic modulus values obtained from the MD results into Eq. (5). The constrain of tangent modulus ($E_t \geq 0$) is adopted to avoid an incorrect material model generated by GA for each trial. Table 4 shows the results obtained from the GA optimization procedure and Figure 8 shows the

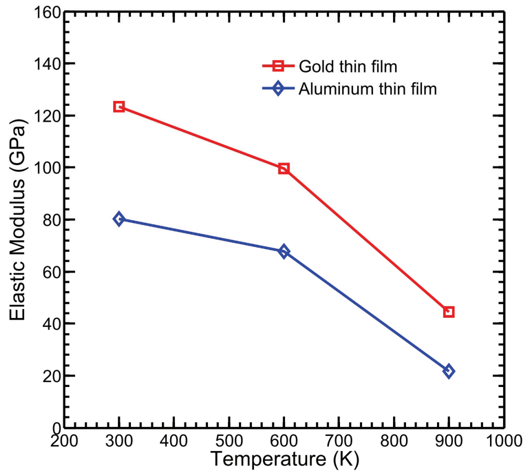


Figure 7: Variation of elastic modulus with temperature as derived from MD load-displacement curves using Oliver and Pharr method [Oliver and Pharr (1992)].

convergence of the population over the generations produced.

Table 4: Inversely-derived material constants by GA

Temperature (K)	Yield stress (MPa)	Tangent modulus (MPa)
Gold film		
300	5461	7265
600	4480	6625
900	2145	279
Aluminum film		
300	4532	848
600	3808	274
900	667	1

These material constants were then used to construct the corresponding stress-strain curves. Figure 9 and Figure 10 presents the inversely-derived stress-strain curves of gold and aluminum films at each of the three test temperatures considered in the MD simulations. Figure 11 illustrates the reduction ratio of the elastic modulus and yield stress, respectively, over the considered temperature range of 300–900 K. From inspection, it is determined that the elastic modulus for the gold and alu-

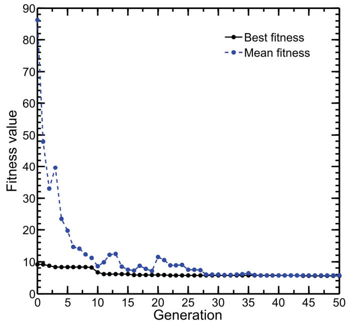


Figure 8: The convergence of population over the generation.

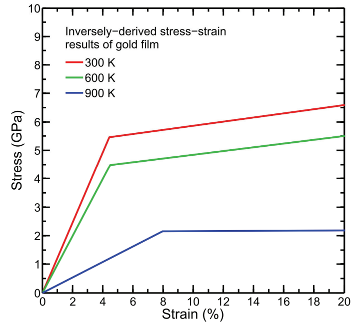


Figure 9: Inversely-derived stress-strain results of gold film at temperatures ranging from 300–900 K.

minum films are approximately 44–123 GPa and 22–80 GPa, while the yield stress for the gold and aluminum films varies from 2.1–5.5 GPa and 0.7–4.5 GPa. Note that the reduction ratio at any temperature is computed simply by dividing the corresponding value of the material property by the value of the property at a temperature of 300 K and then subtracting one. From an inspection of Figure 11, it is found that the elastic modulus and yield stress both reduce more than 15% of their original values as the temperature is increased from 300 K to 600 K. As the system temperature approaches 900 K, it causes thin film weakness and loss of strength more than 60%, as shown in Figure 11.

The value of 80 GPa obtained from the MD simulation for the elastic modulus of aluminum at a temperature of 300 K compares to a value of 77 GPa for aluminum film by direct nanoindentation measurements at room temperature [Pelletier, Krier, Cornet and Mille (2000)]. In other words, the inversely-derived value of the elastic modulus is only around 4% discrepancy than the experimental result. The reported elastic modulus for the gold films was approximately 110–130 GPa [Liu, Fang and Lin (2007)], while it was 123 GPa by the present MD analysis. The validity of the inversely-derived stress-strain curves can be confirmed by using the associated stress-strain data to recreate the corresponding FE load-displacement curves and then comparing these curves with those obtained from the MD simulations. The corresponding results are shown in Figure 12 and Figure 13. Good agreement exists between the two sets of results in every case. The correctness of the inversely-derived stress-strain curves is verified.

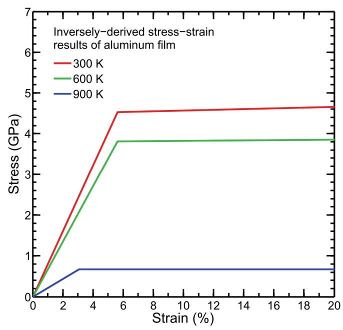


Figure 10: Inversely-derived stress-strain results of aluminum film at temperatures ranging from 300–900 K.

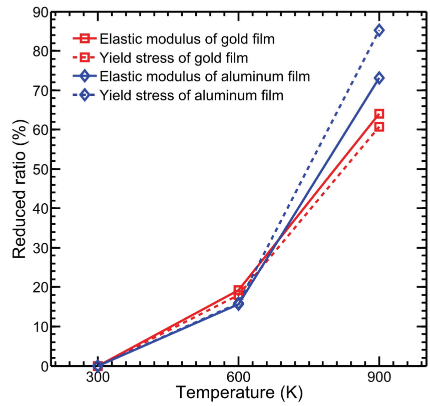


Figure 11: Variation of elastic modulus and yield stress and corresponding reduction ratio over considered temperature range.

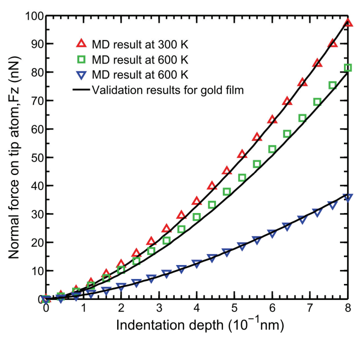


Figure 12: Comparison of FE load-displacement curves based on stress-strain data inversely derived by GA and MD load-displacement curves for gold film.

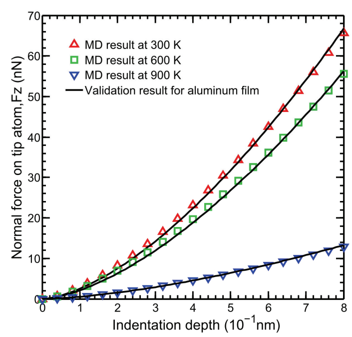


Figure 13: Comparison of FE load-displacement curves based on stress-strain data inversely derived by GA and MD load-displacement curves for aluminum film.

7 Conclusion

This study has proposed a novel method for estimating the temperature-dependent elasto-plastic properties of a nanoindented thin film. In the proposed approach, MD simulations of the nanoindentation process are performed at various temperatures.

The resulting load-displacement curves are then used to identify suitable conditions under which to perform FE simulations of the nanoindentation process. The genetic algorithm (GA) and finite element model (FEM) are used for extracting the material constants of the gold and aluminum substrates. These material constants are used to construct the stress-strain curve, from which the elastic modulus, yield stress and tangent modulus of the indented material are then derived. Finally, the validity of the inversely-derived stress-strain curves is confirmed and the results show that a good agreement exists in load-displacement curves for nanoindentation process. From the proposed inverse analysis method, it is found that the elastic modulus for the gold and aluminum films are approximately 44–123 GPa and 22–80 GPa, while the yield stress for the gold and aluminum films varies from 2.1–5.5 GPa and 0.7–4.5 GPa. The resulting temperature-dependent stress-strain curves provided the crucial requirement for quantitative study of nanofabrication process such as nanoimprint lithography and nanoelectromechanical systems.

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