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Structural and Mechanicals Behaviors of Single Crystals Silicon – Gold Alloy– Atomic Simulation Study

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Abstract

Tensile uniaxial test and simulation dynamic molecular have been used to evaluate the effect of gold (Au) addition and the temperature on the elastic behaviors and structure of Si-Au alloy single crystal. By the following, the interactions are described via a modified embedded-atom model. It has been found that, the yield stress and young modulus decrease when the fraction of atoms Au increases. An increase in the yield stress with temperatures has also been noted. On the other hand, we analyzed the structure of the alloys for high stress. We have shown a dependency of the structure as a function of temperatures.

Keywords: Tensile, elastic behavior, yield stress, temperature, young modulus

1. INTRODUCTION

Many researches interested of Silicon nonmaterial's, because their very interesting optical, electronic and mechanical properties [1-3]. They have good thermal conductivity and are free from thermal fatigue because of their high strength resulting in elastic rather than plastic deformation under stress [4]. In the system Si-Au alloy, the bonding strength is higher than 5.5GPa, when the composition is at the atomic ratio of 81.4% Au [5].Few studies have been performed to characterize the mechanical properties of nanoporous Au obtained by dealloying [6]. The stress at which irreversible deformation initiates, here called the yield stress, was estimated by nanoindentation on nanoporous Au films bonded to a silicon substrate. Dongyun Lee et al [7], studied microfabrication and mechanical properties of nanoporous Au at the nanoscale by finite element analysis and found the elastic modulus of the nanoporous Au is about 8.8 GPa and that the initial yield stress is about 111 MPa and that the ultimate stress at failure due to deformation localization is as high as 190 MPa. Keonwook et al [8] studied tensile of silicon by dynamics molecular (DM) and Modified embedded-atom model (MEAM) potential and found the fracture mechanism of Si nanowires depends not only on the temperature. Yanming et al[9], studied evaluate the surface tensions for the Si supersaturated liquid Si-Au system alloy by DM and potential MEAM and found the surface tension decreases linearly with both increasing temperature and Si fraction. So the surface tension depends on many factors such as the Si fraction and temperature[10,11]. However, the measurement of the surface tension in experiments is usually difficult and the results in literature have a significant variation with different experimental techniques and environment [12] Therefore, estimation from the atomistic simulation would be a necessary complement to the experiments [13]. Typically there is an approached to evaluate surface tension from molecular dynamics simulations namely the mechanical method that extracts the surface tension from the Virial stress [14].

In this work we have studied mechanical and structural behaviors of single crystal alloy Si-Au at different atoms fraction of Au as well as tensile test of Si-Au alloy of 5% Au content at different temperature by DM. The yield stress and Young's moduli were determined at different tests. We have used common neighbor analyses OVITO tools [15] for determinations the structure types of our specimens at high stress.

2. METHODS

- The Modified embedded-atom model

In the MEAM formalism, the potential energy function can be expressed as

$$E = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \# j} S_{ij} \varphi_{ij}(r_{ij}) \right\}$$

Where $F_i(\bar{\rho}_i)$ is the embedding energy function depending on the background electronic density $\bar{\rho}_i$ and φ_{ij} is the pair potential interaction as a function of interatomic distance r_{ij} between atoms i and j, and S_{ij} is a screening factor the MEAM formulation is well document is the literature,[16]

- Molecular dynamic simulations

With this MEAM potential we have performed MD simulation using LAMMPS code to investigate the mechanical and structural behavior of Au-Si alloys at different temperature and fraction atoms addition of Au. For this

purpose, we have created a box (5nm X 5nm X 30nm) of about 104 atoms in the single crystal the structure face centered cubic (FCC). All dynamical simulations are carried out with Varlet's algorithm in the velocity [17], using a time step of 1fs, the specimen prepared 40 ps in a canonical ensemble (NPT), the rate of deformation is 10^{-10} s^{-1}.

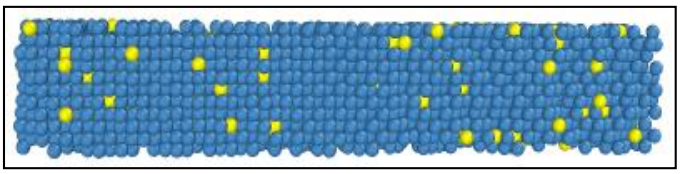


Fig. 1 Example of specimens of single crystal Si-Au alloy of 5% Au content

2.1 Results and discussion

- **Effect of the fraction atoms (Au) on curve stress-strain for single crystal Si-Au alloy**

Fig 2 shows the variation of stress vs strain at different fraction atoms of Si-Au alloys for temperature 300K. We have observed that the yield stress of systems decreases when the fraction atoms of Gold increases. Moreover, the slope of region elastic become stepper. This has been raised by other authors for other systems [8]. On the other hand, we can't see the region plastic in the curve stress-strain but we observed the region elastic and fracture brittle. This shows our system has brittle features.

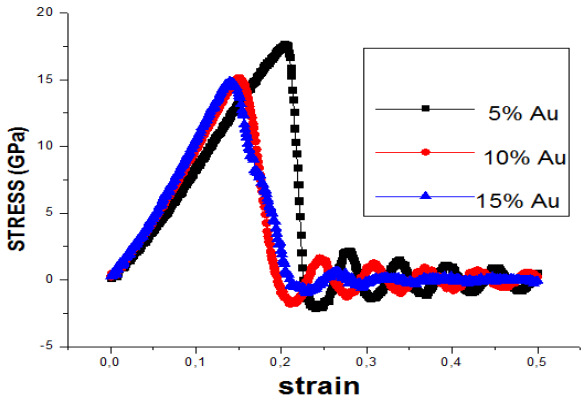


Fig. 2 Evolution of stress vs strain at different fraction atoms of Au

- **Effect of the fraction atoms (Au) on young modulus for single crystal Si-Au alloy**

For study influence of the fraction atoms (Au) on Young modulus E of the single crystal Si-Au alloy, we have fitted the region elastic of curve stress-strain (fig 2). Then, we have plotted the variation of Young modulus as function of the Au fraction atoms (fig 3). We have noted that the young Modulus increases nearly linearly when the fraction atom (Au) increases in the Si-Au single crystal alloy. This result is in good agreement with literature [8].

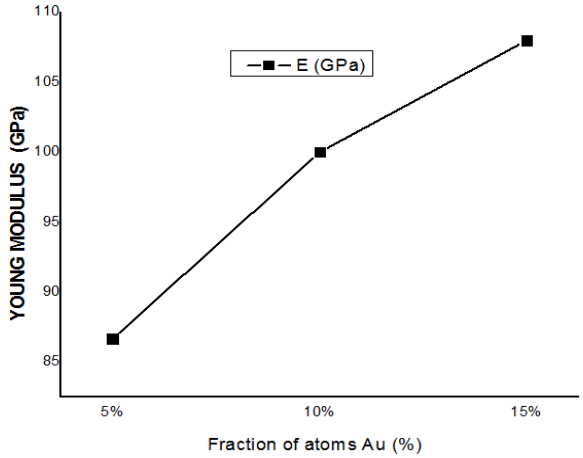


Fig. 3 Young's modulus of Si-Au alloys vs Au content at room temperature

- **Effect of the fraction atoms (Au) on yield stress of single crystal Si-Au alloy**

In order to investigate the effect of fraction atoms on yield stress of the single crystal Si-Au alloys, we have determined the yield stress graphically from figure 2. We have plotted their evolution in term of Au content as shown in figure 4. We observed the values of yield stress decrease when the fraction atom of Au increases. Previous studies on other systems have shown similar trends [8].

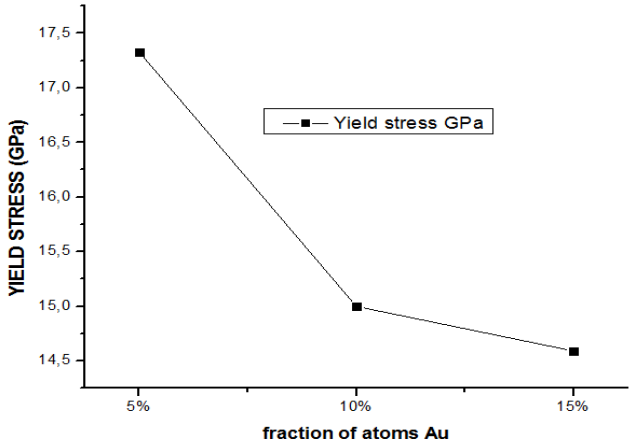


Fig .4 The evolution of yield stress vs fraction of atom Au.

Fig 5 shows the evolution of the curve stress-strain at different temperature. We have observed the yield stress of Si-Au alloy the 5% Au content decreases when the temperature increases. On the other hand, the plastic deformation was observed in the alloy when tested at 500K, due to the free volume induced structural relaxation [18, 19]. This curve exhibits clearly a bent which correlates with the occurrence of a deformation controlled by perfect dislocations. To better discuss this result, we analyzed our samples using the common neighbor

analyses (CAN) tools. The results are organized in the fig 6. We have observed the phase transition at these temperatures without rupture. To know, for 18,5% of BCC, 16% of FCC and 74,3 of other structure, but at low temperature we noted the brittle fracture, thus we can be attributed these results to the phase transition. The same behaviors is observed in single crystal of silicone and system Si-Al alloy [20,21,22,23]

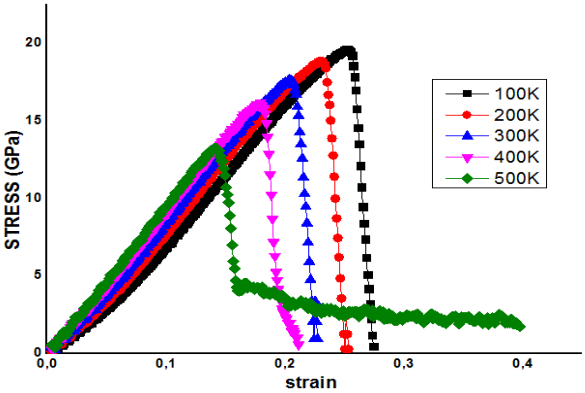
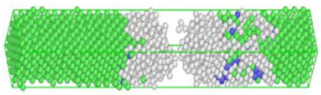
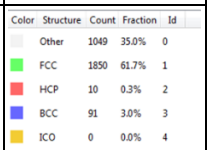
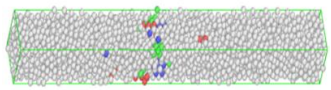
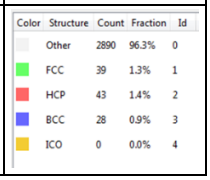


Fig .5 Variation of stress –strain the Si-Au alloy the composition 5% the Au at different temperature.

temperature	picture of specimen at maximum the stress	Structure types
300K		
500K		

5. CONCLUSIONS

The molecular dynamics simulations and the potential MEAM of system Si-Au are used for study tensile of single crystal Si-Au Alloy at different fraction of atoms the Au as well as tensile of Si-Au at 5% Au content at different temperature. The results of our simulation are as follows:

- The yield stress of single crystal Si-Au decreases when the fraction atom of single crystal increases.
- The young's modulus of system Si-Au alloys increases when the fraction of atom Au increases.
- The yield stress of system Si-Au at 5% Au increases when the temperature increases.
- Analyses of specimens at high stress by CAN shown the structure types dependent of temperature.

These results are in good agreement with the literature.

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