136e Structure and Energetics of Gold Breaking Junctions

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The molecular break junction technique is a method for preparing a single molecule bonded to two gold nanowires, a configuration in which it is possible to measure the current-voltage characteristics of a single molecule [1] and involves pulling a gold nanowire apart inside a solution containing the molecule whose properties are to be measured. Clearly, experiments utilizing the molecular break junction technique have relevance to the development of molecular electronics devices. In this talk, we present our studies on the structure and energetic properties of stretching of gold nanowire to breaking point using ‘glue model'- a many-body potential successfully described many features of gold such as bulk, defect and surface properties [2]. Molecular dynamic (MD) simulation has been employed to investigate the effect of initial geometries, crystallographic orientation, elongation rate and temperature on the finial configuration of breaking junctions during elongation process. We found that the final rupture configuration was independent of the initial geometry at fixed temperature. Moreover, investigations of three different crystallographic orientations [001], [110] and [111] combined with the elongation rates ranging from 0.1 m/s to 5m/s reveal that both crystallographic orientation and elongation rate within our MD regime have little effects on the final breaking junction structure. However, elongation of nanowires is quite temperature dependent. The ductile elongation at room temperature is almost two times of that at 0.01 K. Furthermore, in order to understand the mechanical properties of gold nanowires, we calculated the true stress-strain curves for different models during the ductile elongations. After a short elastic response, the yield stress of the neck formed during nanowire breakage remains approximately constant with a magnitude of ~10 GPa. The final true strain can be as large as 50 % before the rupture.

1. Reed, M.A., et al., Conductance of a molecular junction. Science, 1997. 278(5336): p. 252-254. 2. Ercolessi, F., M. Parrinello, and E. Tosatti, Simulation of Gold in the Glue Model. Philosophical Magazine a-Physics of Condensed Matter Structure Defects and Mechanical Properties, 1988. 58(1): p. 213-226.