

Nanowires and Suspended Atomic Chains from Au-Ag Alloys

J. Bettini¹, F. Sato², P. Z. Coura³, S. O. Dantas³, D. S. Galvão², D. Ugarte^{1,2}

¹Laboratório de Luz Síncrotron, 13084-971, Campinas-SP, Brazil

²Instituto de Física, UNICAMP, 13081-970, Campinas-SP, Brazil

³Departamento de Física, UFJF, 36036-970, Juiz de Fora-MG, Brazil

In recent years a large amount of theoretical and experimental work has been carried out on the subject of atomic-size pure metal nanowires (NWs) generated by mechanical stretching [1]. However, it is essential to extend these studies to metal alloy NWs in order to gather information on the mechanical and electrical properties of alloy nanosystems. At the moment rather limited results have been obtained for these structures.

In this work we have used time-resolved high resolution transmission electron microscopy (HRTEM) and molecular dynamics simulations to study the atomistic aspects of the mechanical stretching of Au-Ag NWs of different compositions.

Metal NWs were produced *in situ* in the HRTEM (JEM-3010 URP 300 kV, 0.17 nm point resolution) using the methodology proposed by Kondo and Takayanagi [2]. The Au-Ag alloy thin films (10-30 nm in thickness) were prepared by thermal co-evaporation of both metals in a standard vacuum evaporator (10^{-7} mbar). A quartz crystal monitor was used to set the evaporation rate of each metal source and, subsequently, to measure the equivalent thickness of the alloy films.

In order to obtain more insights on the atomistic aspects associated with the structural evolution of metal alloy NWs, we have also carried out tight-binding molecular dynamics simulations using second-moment approximation (TB-SMA). This methodology has recently proved to be very efficient to study NWs [3,4].

In general terms our studies of metal alloy NWs revealed that, unlike pure metals, structural defects (mainly twins and stacking faults) are sometimes present at the apexes and very close to the narrowest wire constriction, or even in the NW themselves. Similarly to pure NWs we have observed the occurrence of linear atomic suspended chains (LACs). These are the first experimental evidences that LAC formation is possible from metallic alloys (Fig. 1). HRTEM data analysis suggests that these atomic chains are composed of atoms of different types (Au and Ag). Molecular dynamics simulations also present these configurations (Fig. 2).

Another interesting aspect inferred from experiments and simulations is that the atomic-size Au-Ag alloy NWs exhibit a spontaneous gold enrichment of the nanojunction region during the wire thinning process. This leads to a dominant gold-like behavior, even for alloys with minor gold content. This can allow the spontaneous generation of organized Ag core-Au shell structured nanowires or even, in some cases, pure Ag surface enclosing a gold mono-atomic wire. These phenomena open new opportunities to control the stability or length of the atomic chains by a suitable alloy composition.

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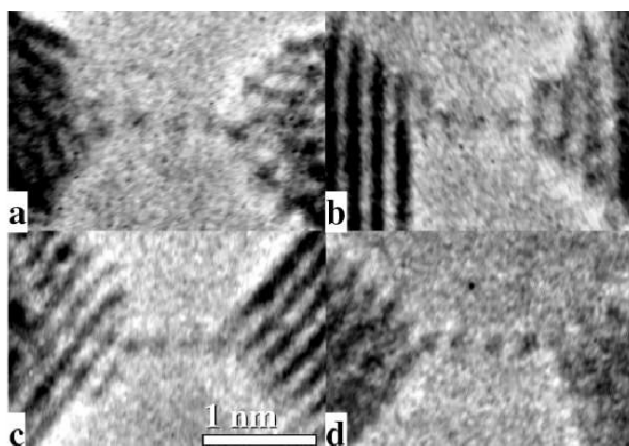


Figure 1. Atomic resolution HRTEM snapshots of suspended atomic chains generated from different alloy compositions $\text{Au}_{1-x}\text{Ag}_x$, for $x=0.2, 0.4, 0.6,$ and $0.8,$ respectively. Atomic positions appear dark.

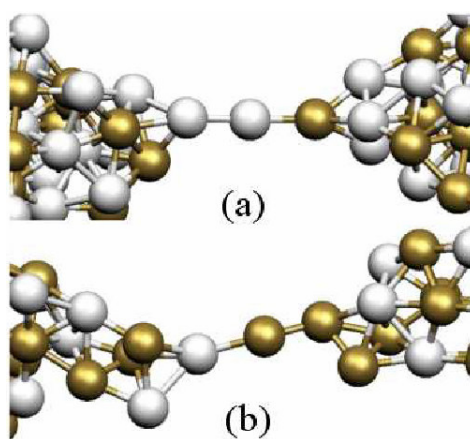


Figure 2. Snapshots from the molecular dynamics simulations showing the formation of mixed linear suspended atomic chains from metal alloys. Yellow (gray) indicate gold (silver) atoms. (a) $\text{Au}_{40}\text{Ag}_{60}$; (b) $\text{Au}_{60}\text{Ag}_{40}$.