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Interatomic force of hexagonal close packed and face centered cubic Co nanowires with different diameters

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ABSTRACT

In this work, the interatomic force of hexagonal close packed (hcp) and face centered cubic (fcc) was studied based on the interatomic interaction potential energy curve using *in-situ* high temperature X-ray diffraction (XRD) in the range of 25–800 °C. The results indicate that the interaction force between atoms for Co nanowires with 45 nm is larger than that for Co nanowires with 55 nm regardless of their hcp and fcc structures. The finding here might be attributed to the surface tension effects, which is of great fundamental and practical significance for the nanodevice application.

1. Introduction

With the development of nanodevices, the studies on the highly ordered arrays of magnetic nanowires including Fe, Co, Ni have been attracting a growing interest [1–4]. The ordered arrays, together with the intrinsic nature of the nanomagnets, can give rise to outstanding cooperative properties which are different from bulk and even film systems such as high-density magnetic memories, magnetic resonance imaging, and magnetically guided drug delivery [5–8]. However, to integrate these magnetic nanowires into complex nanodevices, it is of paramount importance to develop a precise mechanical design criterion based upon the known mechanical properties because mechanical failure of any nano building block may lead to the malfunction or even fatal failure of the entire device. It is known that for the nanomaterials the atoms at or near a free surface reduce coordination relative to interior lattice atoms. This reduced coordination gives rise to surface energy. Although the effect of surface energy on mechanical properties is usually insignificant on a bulk scale, it has been found that surface energy and associated surface relaxations influence the mechanical behavior of nanostructures [9–11]. The effect is realized because the surface area to volume ratio dramatically increases when the size decreases to the nanometer range, and causes a proportional increase in the role of the surfaces during mechanical deformation. It is worth noting that there are very few experimental measurements of mechanical properties of magnetic nanowires, and most values reported in the literature arise from theoretical calculations [12–15]. In our previous work, the mechanical properties of Ni nanowires have been studied by the method of the *in-situ* high temperature XRD [16]. Unfortunately, the discussion of mechanical properties of magnetic nanowires with different structures and diameters is completely lacking in the literature, and this hinders their applications to a great extent in constructing reliable nanodevices. So, in this communication, we can draw the change trend of interatomic interaction potential energy curves for hcp and fcc Co nanowires with the diameters of 45 and 55 nm on the basis of the results of *in-situ* high temperature XRD, and then deduce the relation between the interatomic force of hcp and fcc Co nanowires and the diameters.

2. Experimental

In our experiments, in order to analyze the mechanical properties of Co nanowires we need know the interaction potential energy because the interatomic force F can be calculated from the interaction potential energy $U(r)$ as following [17]: $F = \frac{\partial U(r)}{\partial r}$, where, r is the interatomic distance. It is well known that there exist the attractive

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and repulsive forces between atoms in a crystal. Under the effects of the attractive and repulsive forces, two atoms have the attractive and repulsive potential energies. These two kinds of potential energies are integrated to form the interatomic interaction potential energy which is related to the interatomic distance. Each value of the interatomic interaction potential energy corresponds to two different interatomic distances in the definite range [17]. With the increase of the temperature, the interatomic interaction potential energy will increase, the oscillation amplitude of the atoms will also increase, and the equilibrium position of atoms will change. However, the equilibrium position of atoms is always at the center point between two interatomic distances corresponding to the same interatomic interaction potential energy. The equilibrium position of the atoms can be obtained from the results of lattice thermal expansion on the basis of *in-situ* high temperature XRD [16]. So, hcp and fcc Co nanowires with the diameter of 45 nm and 55 nm can be obtained by the method of the electrodeposition synthesis based on the porous anodic alumina membrane (PAAM). This method is a relatively simple and effective route to prepare the nanowires with the uniform diameter. It is important that the PAAM is chemically stable up to 1100 K and is suitable for measuring the thermal expansion at the high temperature [18]. The PAAM templates with different diameters were prepared according to the two-step anodization method as reported [19]. The electrolyte for the preparation of Co nanowires contained 200 g/L $CoSO_4 \cdot 7H_2O$ and 40 g/L H_3BO_3, and the pH value of solution was adjusted to 5.5 with 1 M H_2SO_4. The detailed electrodeposition process can be found in our previous study [20]. As discussed in our previous work for Ni nanowires with the diameter of 45 nm [16], in order to obtain the intrinsic result, the samples were annealed at 800 °C for 3 h in vacuum of 10^{-3} Pa to remove the vacancies.

The morphologies and the growth orientation of hcp and fcc Co nanowires were characterized with transmission electron microscopy (TEM: JEOL JEM-2100). For TEM observations, the PAAM was completely dissolved with 1 M NaOH solution and then rinsed with absolute ethanol. For XRD measurements, the overfilled nanowires on the surface of the PAAM template were mechanically polished away. To investigate lattice thermal expansion of Co nanowire arrays with hcp and fcc structures, the samples were placed on a Mo holder under high vacuum atmosphere, and measured in the range of 25–800 °C by X-ray diffractometer (Rigaku D/MAX2400) with Cu-Kα_1 radiation ($\lambda = 0.154056$ nm). Before each measurement, the sample was heated to the defined temperature at the increasing rate of 10 °C/min and kept at that temperature for 10 min to stabilize the sample temperature. In our experiments, only the lattice thermal expansion along the axis of Co nanowires was measured.

3. Results and discussion

In the previous work [20], it is reported that, hcp Co nanowires are formed at the low deposition potential, and fcc Co nanowires are formed at the high deposition potential. Here, Fig. 1(a) shows the typical TEM image of hcp Co nanowire with the corresponding selected-area electron diffraction (SAED) pattern, and the corresponding high-resolution transmission electron microscopy (HRTEM) image is shown in Fig. 1(b). It can be seen from Fig. 1(a) and (b) that the diffraction pattern can be indexed to hcp structure, and Co nanowires have a preferred orientation along the [10 $\bar{1}$ 0] direction. Meanwhile, SAED pattern and HRTEM image in Fig. 1(c) and (d) prove that Co nanowires with fcc structure have the preferred orientation along the [110] direction.

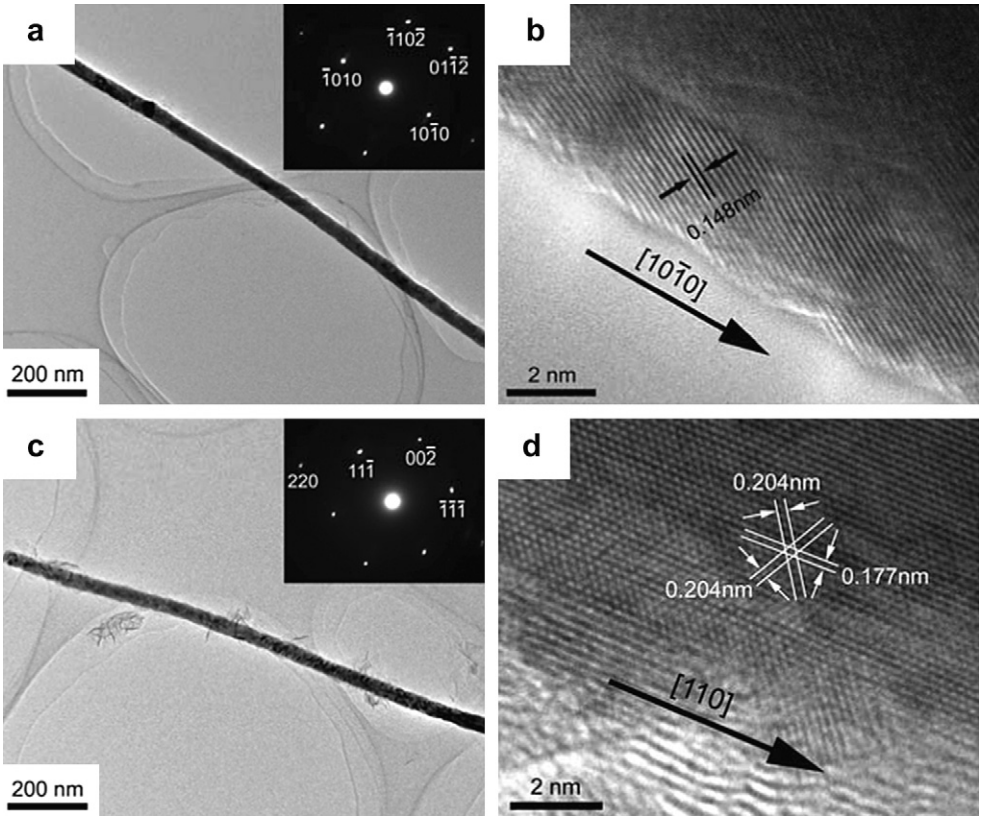

Fig. 1. TEM and HRTEM images of Co nanowires with different structures: (a) TEM image of hcp Co nanowire and SAED pattern, (b) HRTEM image corresponding to the nanowire shown in (a), (c) TEM image of fcc Co nanowire and SAED pattern, (d) HRTEM image corresponding to the nanowire shown in (c).