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Investigation of zirconium nanowire by elastic, thermal and ultrasonic analysis

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Abstract: The elastic, thermal and ultrasonic properties of zirconium nanowire (Zr-NW) have been investigated at room temperature. The second and third order elastic constants (SOECs and TOECs) of Zr-NW have been figured out using the Lennard–Jones Potential model. SOECs have been used to find out the Young's modulus, bulk modulus, shear modulus, Poisson's ratio, Pugh's ratio, Zener anisotropic factor and ultrasonic velocities. Further these associated parameters of Zr-NW have been utilized for the evaluation of the Grüneisen parameters, thermal conductivity, thermal relaxation time, acoustic coupling constants and ultrasonic attenuation. On the basis of the above analyzed properties of Zr-NW, some characteristics features of the chosen nanowire connected with ultrasonic and thermo-physical parameters have been discussed.

Keywords: elastic constants; thermal conductivity; ultrasonic attenuation; Zirconium nanowire.

1 Introduction

Researchers and material scientists are always excited to discover advanced materials with exotic properties which can extrude to the old conventional materials. The development of nanotechnology in earlier phase gives the potential benefits to the material science. Nowadays, nanoscience has become one of the most stimulating forces to influence the interdisciplinary science and technology. The investigations in these areas begin with the understanding of material's behaviour at nanoscale. The attempts were done to control over the crucial physical properties of the materials such as conductivity, capacity, strength, ductility, reactivity etc. in different combination of the matters. This will result in the enhancement of the material's performance at ambient physical conditions. When the size or dimension of a material is continuously reduced from a large or macroscopic size to a size up to 100 nm, the properties remain the same but below 100 nm, dramatic changes in properties can occur [1]. Thus, the bulk properties of the materials become modified when their sizes are reduced to the nano range (1–100 nm). If one dimension is reduced to the nano-range, keeping other two dimensions unchanged, we obtain a structure known as a 'quantum well'. If two dimensions are reduced and one remains unchanged, the resulting structure is referred as a 'nanowire'. The single crystalline NWs are considered as the imperative division of the nanostructure materials due to its superior properties. Currently, the magnetic NWs have drawn considerable interest of researchers worldwide due to their applications in the high-density magnetic storage media, giant magnetoresistance (GMR) sensors [1, 2], bio-magnetic [3], medical devices [4], etc. Among the magnetic nanowires, Zirconium nanowires (Zr-NWs) are widely studied material for its two unusual properties. The first one is the temperature induced phase transformation and the second one is the plastic deformation by twinning. Zr-NWs are the phase changing material and exist in hexagonal close packed (HCP) phase at room temperature (300 K) [5]. Figure 1 shows the HCP structure of the Zr nanowire and its cross-sectional view. Figure 1 clearly indicates that very few Zr atoms are lying on the surface of nanowire in comparison to the volume.

In the field of non-destructive characterization, the ultrasonic non-destructive technique (NDT) has been the most extensively used for the characterization of the materials. The structural inhomogeneities, non-linear elastic properties, phase transformations, electrical properties,

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