

## 58、魏雪霞（北京理工大学）——点载荷对超晶格有限圆柱应变分布及其量子化电子结构影响

传统连续介质力学和量子力学已经分别在宏观和微观领域形成了相对独立的理论研究体系。超晶格材料的研制成功提供了介于宏观连续介质和微观物质粒子之间的典型介观体系。超晶格材料中具有连续介质力学“小尺度效应”和量子力学“大尺寸量子效应”并存的现象。超晶格材料宏观力学性能、微观变形和量子化性质及其关联方面的研究是连续介质力学和量子力学前沿性交叉领域的一个关键基础科学问题。本文首先采用连续介质力学理论研究了点载荷作用下超晶格组分材料硅锆合金圆柱试样中的不均匀应变场和应力场分布。研究方法主要采用 Lekhnitskii 应力函数法, 通过为应力函数提出一个新的解析表达式, 使得所有的本构方程和边界条件都能够精确满足。从而得到了点载荷作用下有限超晶格组分材料硅锆合金圆柱试样内不均匀应变场和应力场分布的精确解析解。然后又从量子力学的薛定谔 (Schrodinger) 方程出发, 采用  $k \cdot p$  微扰方法, 研究了应变对硅锆合金量子化电子结构的影响, 得到了考虑轨道自旋耦合效应和应变效应的量子化电子结构能量的解析表达式。具体分析了应变对硅锆合金量子化电子结构等能面形状的影响。

## 59、张 吟(中科院力学所)——Extracting the Mechanical Properties of 1D Nanostructures from Nanoindentation

The so-called one dimensional (1D) nanostructures or wirelike nanoentities, such as nanowire (NW), nanotube (NT), and nanobelt (NB) have attracted much interest in scientific community because of their remarkable mechanical, electrical, thermal properties and potential applications in wide variety of devices. The mechanical failure of 1D nanostructures can lead to the malfunction or even failure of entire device and 1D nanostructures may also have size-dependent properties. Therefore, an accurate measurement of their mechanical properties is of

critical importance when integrating them into nanodevices. Unfortunately, the experimental measurements of 1D nanostructure mechanical properties are often different and even contradicting to one another. 1D nanostructure is highly flexural due to its large aspect ratio of length to thickness. The bending and lift-off of NB form a localized contact with substrate, which makes the Oliver–Pharr and Sneddon methods inappropriate for 1D nanostructure indentation test. Because the 1D nanostructure/substrate deformation may have significant impact on the force-indentation depth data obtained in experiment, the elastic half-space model assumed by the Oliver–Pharr and Sneddon methods can lead to erroneous predictions on the 1D nanostructure mechanical properties. 1D nanostructure in indentation test can be susceptible to the adhesion influence because of its large surface area to volume ratio. 1D nanostructure/substrate contact and adhesion can have direct and significant impact on the interpretation of experimental data. The influence of 1D nanostructure/substrate contact and adhesion is analyzed and methods of reducing such influence are also suggested.

#### **60、张俊杰（哈尔滨工业大学）——机械纳米加工过程的原子模拟**

机械纳米加工技术可以获得具有特定形状的三维纳米结构。使用基于分子动力学的原子模拟方法研究了单晶铜、多晶铜的机械纳米加工过程，重点关注了加工过程中材料变形机理，如位错滑移、变形孪晶，位错与晶界的交互作用，以及力学与摩擦学性质。研究发现单晶铜的变形主要是通过位错形核及滑移来实现，而变形孪晶是多晶铜的一种重要的变形机理。晶界阻碍加工过程中位错运动，从而影响已加工表面质量。