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Review Article

Effect of lattice strain on nanomaterials in energy applications: A perspective on experiment and theory

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ABSTRACT

Nanostructured semiconducting materials such as nanoparticles, quantum dots, nanowires, nanorods, nanotubes, nanobelts, nanoribbons, nanosheets, nanolayers, nanofilms, etc have gained tremendous attention within the past decade due to their fascinating physical properties and potential technological applications in electronic and optoelectronic devices. Semiconducting materials are able to be altered with strain-inducing from tunable sizes and shapes due to quantum confinement effects. Lattice strain is found to be very useful as well as very economical methods for improving the performance of energy devices by modifying band structure of nanostructured materials. The use of strain in design of nanostructured semiconducting materials is now a standard technique for modulating their electronic structures to enhance both electron and hole mobilities. There are mainly three effects of strain on nanostructures: (i) electronic band modulation, (ii) buckling, and (iii) phase transformations. In this review, we mainly focus on both experimental and theoretical achievements for effect of strain in nanostructured materials. Finally, the review is concluded with perspectives regarding the effect of strain in low dimensional nanostructured semiconducting materials, particularly zero-, one-, and twodimensional nanostructures in future.

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Contents

Introduction	00
What is a nanostructure?	00
Types of nanostructures	00
Why nanoscale?	00
Experimental achievements for effect of strain on nanomaterials	00
Theoretical achievements for effect of strain on nanomaterials	00
Summary and perspectives	00

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Acknowledgement	00
Acronyms used in this review	00
References	00

Introduction

The use of non-renewable energy sources worldwide leads to the depletion of these natural sources worldwide in a foreseeable future. At the same time, when these fuels are used for producing high energy, emission of green house gases result in global warming that cause the climate change, flooding, etc. To overcome these problems, the worldwide scientists have been developing the alternate renewable energy sources for sustainable human activities. In this regard, renewable energy sources such as mechanical [1], heat [2], and solar energies [3,4] are being actively investigated. Among all alternatives, solar energy is the most fascinating one as it is emitted from the sun primarily as electromagnetic radiation in the ultraviolet to infrared and radio spectral regions. Basically, solar energy can be harvested in the form of biomass, heat, and electricity. Conversion of sunlight directly into electricity compared to biomass and heat has the highest theoretical efficiency and flexibility. Therefore, solar energy can be harvested by using techniques such as photovoltaics (PVs), photoelectrochemical cells (PECs), and solar hydrogen. To date, the efficiencies of typical commercial solar cells are approx. 24.7% (claimed by Panasonic) for single-crystal silicon-based PVs, approx. 17.5% for TiO2 based dye-sensitized solar cells [5] and approx. 22% for solar hydrogen production [6]. The cost reduction in device processing and improvement in energy conversion efficiency of the solar cells, photoelectrochemical cells and other electronic devices were achieved using nanostructured semiconductor materials due to the progress of nanotechnology.

What is a nanostructure?

A nanostructure is any structure with one or more dimensions measuring in the nanometer (10^{-9} m) range. For example, polycrystalline materials with nanometer sized crystallites, materials with surface protrusions spatially separated by few nanometers granular or porous materials with grain sizes in nanometer range or nanometer sized metallic clusters embedded in a dielectric matrix. Experimentalists now have access to a huge arrays of nanostructures both self-assembled (e.g. fullerenes, nanotubes, etc.), and directly fabricated (e.g. quantum wires, lateral quantum dots, etc.). These nanostructures are shown as in Fig. 1(a-e).

Types of nanostructures

Nanostructured materials are classified according to the dimensions of their structural elements as zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and threedimensional (3D) nanomaterials.

Zero-dimensional nanomaterials include nanoparticles or well-separated nano-powders with nanometric size range, i.e. nanoparticles are isolated from each other. One-dimensional nanomaterials have a certain shape such as nanorods, nanowires, nanotubes, and nanoneedles. Two-dimensional nanomaterials have plane shape such as film (coatings) with nanometer thickness. For example, nanofilms, nanocoatings, and nanolayers are 2D materials. Three-dimensional nanomaterials include powders, fibres, multilayers, and polycrystalline materials in which 0D, 1D and 2D structural elements are in close contacts with each other and form interfaces. Therefore, 3D nanostructures contain various groups of nanoparticles, nanocrystallites, nanowires, nanotubes, and nanolayers. All 0D, 1D, 2D and 3D nanostructures can be amorphous or nanocrystalline. In case of 3D nanostructure, it is a compact or consolidated (bulk) polycrystal with nanosize grains in which grain surface is absent and there are only grain interfaces. These nanostructures are shown as in Fig. 2 [7].

Why nanoscale?

The materials can be divided into two types: (i) Brittle and (ii) Ductile. In bulk size, due to existence of crack (for brittle materials) or dislocation (for ductile materials), materials can not sustain large strain. Brittle materials fracture at very small strain due to stress concentration around the crack, and ductile materials plastically deform by the dislocation motion. When materials become nanoscale, the crack size becomes very small for brittle materials and the dislocation density becomes very small for ductile materials. Hence, nanomaterials can sustain homogenous high electric strain without failure or yield. For example, Si NWs were found to exhibit an enormous range of elastic strain up to 12% [8], which is promising for elastic strain engineering. In addition, Welser et al. [9,10] were among the first to demonstrate a



Fig. 1 – Nanostructures (a) fullerene, (b) nanotube, (c) nanowire, (d) graphene nanosheet, and (e) square-pyramid nanostructures.

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