International Research Journal of Advanced Engineering and Science
ISSN (Online): 2455-9024

The Structure and Mechanical Properties of Nanocrystalline Materials Specially used in Solar Cell - A Review

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The present article reviews the current status of research and development on the structure and properties of nanocrystalline materials used in solar photovoltaic cell material with its mechanical properties. In this study the size of materials of Nanocrystalline materials with different grain sizes taken into consideration. Because of the different size of materials with dimensions effect a large fraction of the atoms in these materials is located at the grain boundaries, and this confers special attributes. Nanocrystalline materials can be prepared by inert gas-condensation, mechanical alloying, plasma deposition, spray conversion processing, and many other methods.

The nanocrystalline semiconductor of group II-VI, III-V, IV-VI has been widely used in photovoltaic cell, solar cell, LED and sensors. These nanocrystalline semiconductors are easy to synthesise in a prerequisite dimensions and also contain large number of surface atoms .Zinc oxide (II-VI) is also an interesting semiconductor with direct band gap of 3.3 eV and excitonic binding energy (60 meV). Nowadays ternary semiconductor like ZnCdS show excellent physical properties for application in window layer of solar cell, low voltage cathode, luminescence, electroluminescence displays and anti-reflection coating for infra-red devices. These semiconductors have wide energy gap lying between CdS (2.4eV) and ZnS (3.68eV). And by changing the percentage of Zn:Cd ratio the band gap of ZnCdS film can be altered . Many techniques can be followed for ZnCdS thin film deposition like sputtering, spray pyrolysis, vacuum evaporation, chemical vapour deposition (CVD) and chemical bath deposition (CBD).Researchers have prepared nanocrystalline ZnCdS in nonaqueous medium by CBD technique. CBD technique is cheap, simple, uniformly coats and it easily coats larger area. It also gives liberty in choosing sources of deposition, working in higher temperature, free from evolution of ubiquitous hydrogen during reaction and free from pinhole deposition. In this experimental study we have varied the Zn concentration (x = 0.2,0.3,0.4,0.5) and we have studied the effect of Zn doping on morphological, structural and optical properties. The purpose of the present article is to present a very broad overview of the structure and properties of nanocrystalline materials. However, there is no comprehensive review related to the materials aspects; this review is an attempt to fill that gap.

Ductility:-Conventionally in grain size regime, reduction in grain size leads to increase in ductility. However for grain sizes less than 25 nm ductility is very small. The molecular dynamical simulation is considered as a valuable tool in aiding our understanding of deformation mechanism. There are actually three regimes a) grain size d>l µm regime in which unit dislocations and work hardening control plasticity; (b) smallest grain size d < 10 nm regime, where limited intra-granular dislocation activity occurs and grain-boundary shear is believed to be the mechanism of deformation;(c) the intermediate grain size regime (10 nm–1µm) is less well understood. These mechanisms are thought to affect ductility significantly.

By comparison, ultrafine grained materials (100–500 nm), it exhibit increased yield strength along with good ductility in comparison to nano grained materials. To enhance ductility non equilibrium grain boundaries have been proposed, as such boundaries provide a large number of dislocations for slip and also enable grains to slide or rotate that further leads to increase in strain hardening exponent. By decreasing the strain rate also we can increase the ductility. There are three factors that contribute to determine ductility, they are work hardening, strain rate sensitivity and thermal softening. The strain rate sensitivity ‘m’ can be expressed as $m=3^{1/2}kT\backslash V\sigma_y$

Where V is activation volume for plastic deformation, T is the temperature and σ_y is the yield/flow stress.

Inverse Hall –Petch effect: fact or fiction:-The Hall–Petch relationship predicts that the yield stress increases with the inverse of the square root of the grain size. Although experimental results on materials reveal that the Hall–Petch relationship recorded at large grain sizes cannot be extrapolated to grain sizes of less than 1µm.While some results predict a plateau, others show a decrease. There is a lot of differences in trend of plot as grain size falls below 25nm. Although Chokshi et al.were the first to report the negative Hall–Petch effect by performing measurements on nanocrystalline Cu and Pd samples made by IGC. Both metals exhibited a negative slope, shown in Fig. below. They attributed this negative trend to diffusional creep in nanocrystalline samples at room temperature analogous to grain-boundary sliding in conventionally-grained samples at high temperature.

Shreoshi Dasgupta, D. N. Mahato, and M. K. Paswan, “The structure and mechanical properties of nanocrystalline materials specially used in solar cell - A review,” *International Research Journal of Advanced Engineering and Science*, Volume 3, Issue 4, pp. 100-102, 2018.

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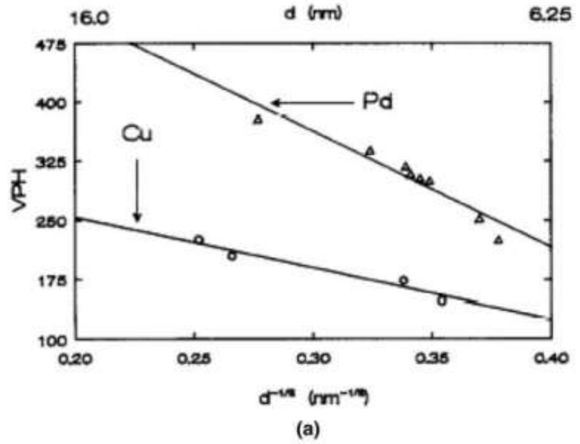

Fig. (a). Inverse Hall Petch effect trend For Cu Pd as shown by Chokshi et al.

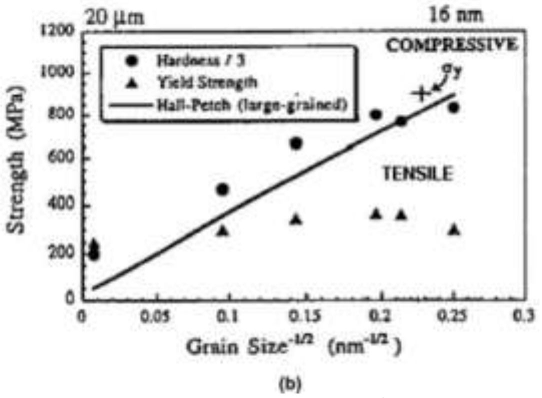

Fig. (b). Positive Hall Petch slope with higher values for compressive than for tensile strength.

Strain hardening:-Unlike response of coarse grain polycrystalline material nanocrystalline and ultrafine grained materials cannot generally sustain uniform tensile elongation. They basically show no strain hardening over a small plastic strain regime.

The stress strain response of nano crystalline metal under tension shows a rapid peak and thereby softening due to necking. Necking is observed in most of the cases with severe case of instability.

Strain rate sensitivity:-There are reports stating increased and decreased strain rate sensitivity with decreasing grain size in metals. A different effect was found by Gray et al. On ultrafine grained FCC metals produced by ECAP. Results by Wei et al. shows strain rate sensitivity increases with increase in grain size below a critical value.

Strain-rate sensitivity of ultrafine grained and nanostructured HCP metals:-The effects of temperature, strain rate and grain size on the flow behaviour of Zn (representative HCP metal) have been studied to reveal the deformation mechanisms in UFG and nano crystalline HCP structured metals. It was experimentally found that the grain size after 3 h ball milling was 238 nm. The strain hardening under quasistatic conditions in samples that were tested at different temperatures was low and at 200^0C, it ceased to exist. This in turn leads to an increase in yield stress and a decrease in work hardening.

Mechanical behaviour of iron as a representative BCC metal:-From the plot of stress strain curve it suggest that strain hardening decrease with decreasing grain size. This is probably because of change in deformation mechanism at smaller grain sizes. Jia et al used a physically based constitutive model that describes the rate-dependent behaviour of BCC iron over the entire range of strain rates from 10^{-4} to 10^4s.

Creep of nano crystalline materials:-Creep in coarse grained materials has been widely studied for approximately one century. Creep in nanocrystalline particles have been an interest of researcher after several complication which arised recently i.e to explain deformation process in bulk nanoparticles. Since the volume fraction of grain boundaries is high, diffusion creep is considered to be significant. Ogino attributed the effect to an increase in grain-boundary area due to deformation of grains at an initial stage of creep. Wang et al. studied the effect of grain size on the steady state creep rate of nanocrystalline pure nickel that was synthesized by electrode position.

Fatigue of nanocrystalline materials:-The fatigue life, as measured by S –N (Wo¨ehler) type plots, is enhanced for nanocrystalline metals by virtue of their higher yield stress. On the other hand, ΔK_{th} decreased and da/dn is increased for nanocrystalline metals. This latter effect is because of the smoother fracture path in nanocrystals.

Mechanical Properties of nanocrystalline metals and alloys:-The variation in grain size strongly governed mechanical property of nanocrystalline metals and alloys. With the decrease in grain size, tensile strength and fatigue unit increase in microcrystalline regime. Nanocrystalline metals and alloys with average range of grain size typically smaller than 100nm have been a subject of interest in recent years. The processing of materials and advances in computational technique are being the major reasons of interest in recent years. These material also possess appealing mechanical properties such as high tensile strength, increasing strength and ductility with increase in strain rate, increasing resistance to tribiological environmentally assisted damage and ability for enhanced superplastic deformation at lower temperature and faster strain rate. Nanocrystalline semiconductors are easy to synthesise in a prerequisite dimensions and also contain large number of surface atoms. Nowadays ternary semiconductor like ZnCdS show excellent physical properties for application in window layer of solar cell, low voltage cathode, luminescence, electroluminescence displays and anti-reflection coating for infra-red devices. These semiconductor have wide energy gap lying between CdS (2.4eV) and ZnS (3.68eV). And by changing the percentage of Zn:Cd ratio the band gap of ZnCdS film can be altered

Yield Strength:-Yield strength is the stress at which material begin to deform plastically and will not return to its original shape when applied stress is removed. The theoretical yield strength can be estimated by considering the process of yield at atomic level. Yield strength testing involves taking a small sample with affixed cross section area and then pulling it with a control, gradually increasing the force until the sample changes shape or breaks. This is called tensile Test.

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Longitudinal or Transverse strain is recorded using mechanical or optical extensor vectors.

Diffusion and heating without Melting -Since nanocrystalline materials contain a very large fraction of atoms in different size and dimensions at the grain boundaries, the numerous interfaces provide a high density of short circuit diffusion paths. Consequently, they are expected to exhibit an enhanced diffusivity in comparison with crystals or conventionally available grained polycrystalline materials with the same type of composition.

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