IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Microstructures and characteristics of nano-size crystalline silicon films

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1992 J. Phys.: Condens. Matter 4 L509

(http://iopscience.iop.org/0953-8984/4/40/001)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.96
The article was downloaded on 11/05/2010 at 00:37

Please note that terms and conditions apply.

J. Phys.: Condens. Matter 4 (1992) L509–L512. Printed in the UK

LETTER TO THE EDITOR

Microstructures and characteristics of nano-size crystalline silicon films

L C Wang, D Feng, Q Li, Y L He and Y M Chu

National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210008, People's Republic of China

Received 3 August 1992

Abstract. Microstructures and characteristics of nano-size hydrogenated crystalline silicon films (nc-Si:H) have been studied by high-resolution electron microscopy (HREM), x-ray diffraction patterns and Raman spectroscopy. The microcrystalline grains in nc-Si:H films are about 3–5 nm in size and are separated by different characteristic boundaries. The volume fraction of the crystalline component is about 46%. Micro-defects in nanocrystalline grains were also found. The electrical conductivities of the films were found by measurement to be about 10^{-3}–10^{-2} $(\Omega\ \mathrm{cm})^{-1}$. Analysis of the experimental results shows that the nano-size hydrogenated crystalline silicon films are in good agreement with the international definition of nanocrystalline material.

The crystal structures, growth mechanisms, oxidation and doping of polycrystalline silicon thin films are quite different to those of single-crystal silicon, and are very effective in many devices. In the last ten years or so, polycrystalline silicon thin films have been widely used in integrated circuits, solar cells and sensors; this has brought about improvements in the design and technology of these devices [1–3]. However, microcrystalline silicon thin films are characterized by a series of unusual properties which have interested a lot of researchers [4–6]. Studies have demonstrated that the increase of electrical conductivity in microcrystalline silicon thin films is strongly related to the volume fraction of the microcrystalline phase and its grain size. In this letter, we report the microstructures and characteristics of nc-Si:H films whose electrical conductivity approaches 10^{-3}–10^{-2} $(\Omega\ \mathrm{cm})^{-1}$.

The nc-Si:H films were prepared by a conventional plasma-enhanced chemical vapour deposition (PECVD) system with hydrogen-diluted silane as the reactive gas activated by RF + DC double power sources. A detailed description of the nc-Si:H films prepared has been given elsewhere [7]. The microstructures of nc-Si:H films were directly observed at the atomic level by using a JEM-4000EX electron microscope operated at 400 kV with a point-to-point resolution of 1.9 Å, and C_s = 1 mm. The properties of the samples were characterized using x-ray diffraction patterns (Cu Kα, λ = 1.54 Å) and Raman spectroscopy.

A HREM image of the nc-Si:H films in figure 1 shows that fine microcrystallites had been formed. The arrangements of microcrystallites are irregular, with a mean size of about 3–5 nm; the microcrystallites are separated by boundaries with different atomic structures depending on the orientation relationship between adjacent crystals and the boundary inclination [8]. The structures of microcrystallites have been distorted near

0953-8984/92/400509+04$04.50 © 1992 IOP Publishing Ltd

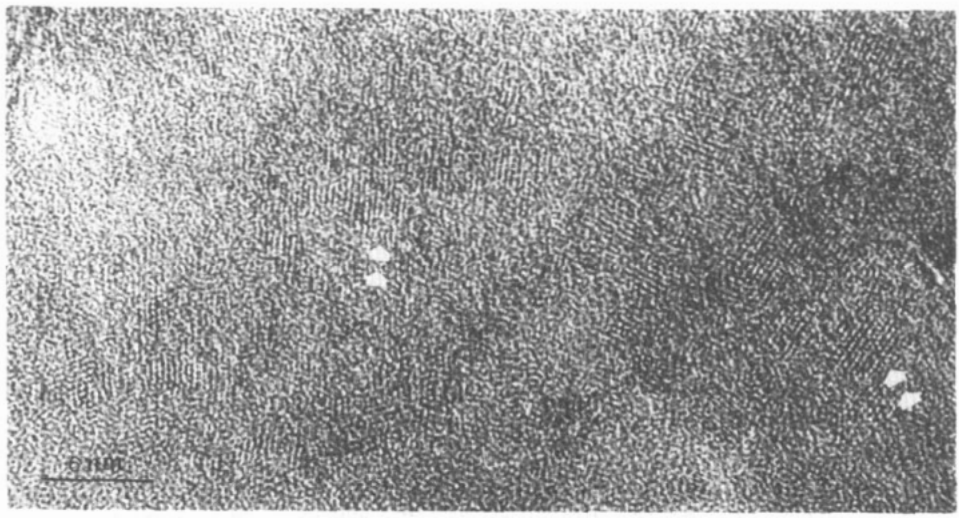

Figure 1. A high-resolution electron microscopy image of the nano-size hydrogenated crystalline silicon films.

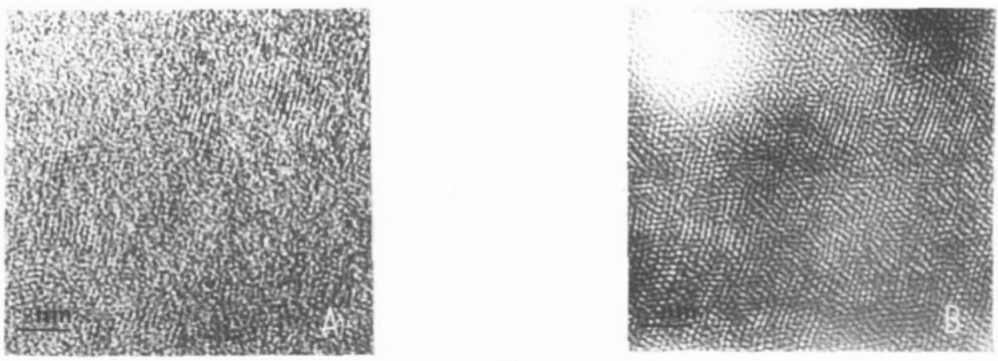

Figure 2. (A) A part image of figure 1. (B) A filtered image of (A)

the periphery, which suggests a strong interaction between the nanocrystalline grains and the boundary. In the central region of microcrystallites, the periodic structures remained relatively intact, but the lattice spacing between close-packed planes became larger than that of single-crystal Si, as measured by means of x-ray techniques. It is considered that the binding forces between atoms within the close-packed planes are much stronger than the binding forces between atoms in adjacent close-packed planes. The micro-defects in nanocrystalline grains have been found, and these are indicated by arrows in figure 1 [9, 10]. In order to make the microcrystallites of the nc-Si:H films clearly visible in the HREM image, digital image processing was performed using an electronic digitizing camera (Hewlett–Packard Scanjet Plus Scanner, Hewlett–Packard Company, USA) and a computer (Model 486/33, Legend Computer Group Company,

China). Figure 2(B) is a filtered image of figure 2(A), which is a part image of figure 1; the characteristics of the grains and their boundaries were observed simply with the disorder component in the background suppressed. The x-ray diffraction pattern in figure 3 was measured for the nc-Si:H films. Diffraction peaks corresponding to the (111) and (220) planes were observed. Using Scherrer's formula, the average size of the microcrystallites was calculated from the half-width of the (111) diffraction peak provided in the x-ray diffraction pattern and was found to be 3.5 nm. The diffraction angle of the (111) plane was shifted towards the low-angle side from $2\theta = 28.47°$ for single crystal to 28.00–0.05° for the nc-Si:H film. The calculated spacing of the (111) plane for the nc-Si:H is 3.166 Å—about 1% larger than that of single-crystal Si (3.14 Å). Figure 4 is a Raman spectrum of nc-Si:H films, which exhibits peaks at 480 cm^{-1}—which is characteristic of disordered Si—and at 515 cm^{-1}—which is characteristic of crystalline Si. The volume fraction of the crystalline component, $f =$ 46%, was obtained from the Raman-integrated intensity ratio of the peaks at 480 cm^{-1} and 515 cm^{-1} using the equation $f = I_c/(I_c + I_a)$; here, I_c and I_a represent the peak-integrated intensity for crystalline Si and disordered Si, respectively. Using the equation $d = 2\pi(B/\Delta\omega)^{1/2}$ the grain size has also been calculated to be 3 or 4 nm from the shift of the microcrystalline peak as compared with the peak at 521.5 cm for single-crystal Si. The calculated values of the grain size are consistent with the result obtained from x-ray diffraction. From HREM, Raman and x-ray techniques, it is confirmed that the average size of the microcrystallites is 3–4 nm, and the volume fraction is 46%. The widths of the boundaries between the microcrystallites were estimated to be about two or three atomic layers from the percentage of the boundary layers. The characteristic values were determined for three kinds of sample and are summarized in table 1 [7]. It is shown that the electrical conductivity of sample 3 is nearly 10^{-3}–10^{-2} $(\Omega\ cm)^{-1}$; this reveals that the high electrical conductivity for the nc-Si:H film was obtained when the volume fraction of the crystalline component increased and the grain size change was small.

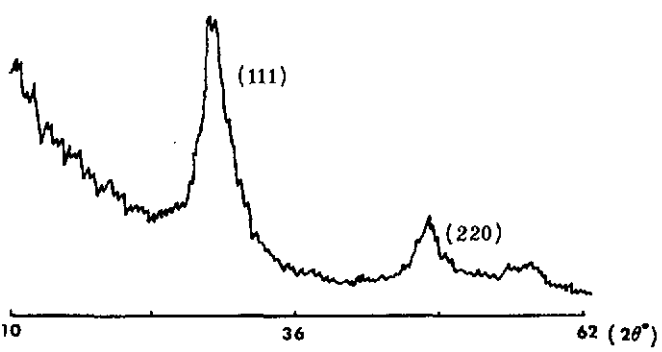

Figure 3. The x-ray diffraction pattern of the nano-size hydrogenated crystalline silicon films.

Our conclusions are that nc-Si:H films with electrical conductivities of 10^{-3}–10^{-2} $(\Omega\ cm)^{-1}$ have been produced by the PECVD method; unusual microstructures of the film were observed; the mean grain size was about 3–5 nm; the volume fraction of the crystalline component was 46%; micro-defects were found in nano-size grains; and the lattice spacing of the close-packed (111) planes was elongated by the strong

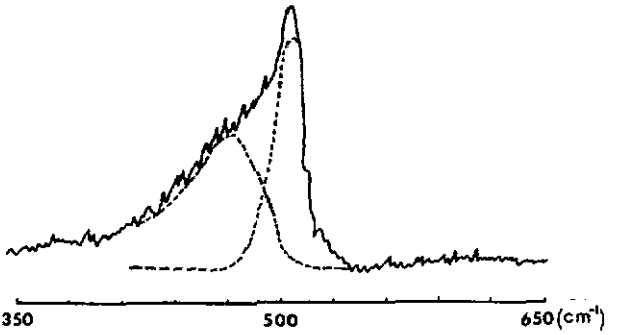

Figure 4. The Raman spectrum of the nano-size hydrogenated crystalline silicon films.

Table 1. Characteristic values of three sample types.

Number of specimens	Grain size (nm)	Volume fraction of crystalline component (%)	Dark conductivity $((\Omega\ cm)^{-1})$	Photo-conductivity $((\Omega\ cm)^{-1})$	Activation energy (eV)
No 1	0	0	4.8×10^{-10}	2.5×10^{-7}	0.73–0.94
No 2	5	0.38	1.7×10^{-4}	1.8×10^{-4}	0.15–0.27
No 3	3–5	0.46	4.3×10^{-3}	4.1×10^{-3}	0.07–0.21

interaction between the grain and its boundary. These results were determined from HREM, x-ray and Raman spectroscopy analysis. The experimental results for the nano-size crystalline silicon film are in very close analogy with the international definition of nanocrystalline material [11–12].

The authors would like to thank Dr S D Yu, J G Zheng, J M Zhu, H P Xu, F Yu and M Wei for useful discussions and assistance. This research was supported by the Nation Natural Science Foundation of China.

References

[1] Zook J D 1980 *Appl. Phys. Lett.* 37 223
[2] Schaber H, Cutter D and Obermeier E 1983 *J. Appl. Phys.* 54 8
[3] Ashburn P and Soerowirdjo B 1984 *IEEE Trans. Electron. Devices* **ED-31** 853
[4] Mishima Y, Miyazaki S, Hirose M and Osaka Y 1982 *Phil. Mag.* B 46 1
[5] Veprek S, Iqhal Z, Kuhne R O, Capezzuto P, Sarott F-A and Gimzewski J K 1983 *J. Phys. C: Solid State Phys.* **16** 6241
[6] Matsuda A, Nomoto K, Takeuchi Y, Suzuki A, Yuki A and Perrin J 1990 *Surf. Sci. (Netherlands)* **227** 50
[7] He Y L, Liu X N, Wang Z C, Cheng K S and Wang L C 1992 *Sci. Sinica* **8** 876
[8] Zhu X, Birringer R, Herr U and Gleiter H 1987 *Phys. Rev.* B **35** 9085
[9] Feng D 1987 *Physics of Metals* vol 1 (Beijing: Science)
[10] Nabarro F R N *Dislocations in Solids* vol 2 (New York: North-Holland)
[11] Gleiter H 1990 *Phase Transitions (UK), Part 1* B **24–26** 15
[12] Gleiter H 1989 *Europhys. News (Switzerland)* **20** 130