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Research Article

Cadmium telluride for high-efficiency solar cells

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Abstract

Problems of the synthesis of cadmium telluride powders having required purity and grain size distribution for high-efficiency solar cells have been analyzed. A test batch of powders has been synthesized and used for the manufacture and study of thin-film solar cell specimens exhibiting parameters compliant with the best worldwide standards. The phase composition of the powders has been studied using X-ray diffraction. Structural analysis and elemental composition measurements have been carried out using electron microscopy. The effect of free tellurium phase in the powders on the endurance of devices manufactured from the powder has been described. We show that excess tellurium in the film specimens whose atoms are predominantly localized along grain boundaries may cause temporal degradation of the electrical properties of the manufactured solar cells due to changes in the parameters of the crystalline structure of the cadmium telluride phase which are caused in turn by changes in the stoichiometric composition of the material. Structural studies of the film specimens have not revealed differences in the film structure before and after endurance tests. A new cadmium telluride powder process route has been developed, proven and tested taking into account the advantages and drawbacks of the previously used process and experiments confirming the correctness of the technical solutions chosen have been conducted.

Keywords

powders, cadmium telluride, thin films, sputter deposition, solar cell, phase composition, elemental composition

1. Introduction

It is well known that the power industry is the basis for the development of the worldwide economy, but the carbon resources on which it still depends are not unlimited, and their production, transportation and processing are becoming increasingly expensive and exacerbate existing environmental problems [1]. Possible solution to this situation is the design, implementation and development of advanced science-based energy conversion and storage technologies on the basis of fundamentally new highly efficient and innovative technical products [2, 3].

One of these promising energy industry development trends is the manufacture of solar photovoltaic devices which over the recent 15 years has been significantly outpacing any other industries worldwide [4, 5]. It should be noted that solar energy production already exceeds 3% of the worldwide generation, with 113 and 129 GW energy production premises put into operation in 2018 and 2019, respectively, thus raising the overall energy production to above 650 GW [6]. However the cost of solar photovoltaic devices is still relatively high as compared with other conventional generation techniques in spite of permanent cost reduction. This cost reached \$69/MWh in 2019 in Europe against the average heat and nuclear plant generated power cost of ~\$50/MWh [4]. Yet, the contract price under many solar energy contracts world over was as low as below \$30/MWh in 2016 which was accounted for by analysts as a consequence of some local economic factors [7].

More than 90% of current solar cell manufacturers worldwide use silicon as the main material [4]. However there are other materials showing good promise for this industry, such as cadmium telluride (CdTe), the efficiency of solar cells on its basis being attributed primarily to the high absorption coefficient and the optimum band gap of the material which is 1.5 eV [8–10]. It should be noted that the electrical properties of CdTe and hence the parameters of solar cells (SC) on its basis are controlled by intrinsic point defects and even minor deviations from the stoichiometric composition [11–14]. Therefore innovative works on CdTe are of special importance. The research into CdTe thin-film high-efficiency SC shows good progress and opens opportunities for an up to 60% solar CdTe solar cell energy cost reduction in the near term thus making CdTe solar cell energy cheaper than that produced with silicon photovoltaic converters [2].

According to the US National Renewable Energy Laboratory (NREL) the highest efficiency of CdTe thin-film SC achieved by FirstSolar, the world's leading solar cell manufacturer, was 22.1% in 2021 [15]. FirstSolar also holds the former 2016 record of 21.5%. FirstSolar's CEO stated the company's goal as to confirm the permanent competitive advantage of CdTe over the conventional single crystal silicon technology.

A typical structure of a CdTe SC is shown in Fig. 1 [9]. The main SC manufacturing processes are sublimation, chemical sputter deposition, chemical vapor deposition (CVD), epitaxy and screen printing [16–20].

In consideration of the foregoing, the research into the problems related to intense development of solar energy and SC-produced energy cost reduction has a global scale and is of a great importance. It is therefore necessary to develop new technical trends which can potentially increase the efficiency of solar photovoltaic devices thus improving their parameters and reducing the cost per 1 W of solar energy.

The aim of this work is to develop technical fundamentals for synthesizing CdTe powders having required stoichiometric composition, grain size distribution and elemental purity for the manufacture of high-efficiency thin-film SC, and to study their properties.

2. Experimental

The test batch of CdTe powder was synthesized by ADV Engineering JSC for Calyxo Co., Germany's leading manufacturer of high efficiency CdTe thin-film solar cell and supplier of turn-key photovoltaic systems. The CdTe powder was synthesized using the standard process used at ADV from at least 5N purity raw components produced following a ADV's proprietary technology [21–24]. The powder was produced in a quasi-air-tight quartz reactor using the direct synthesis process which includes the stages of sintering, annealing, crushing and screening of the synthesized material subject to the customer's purity and grain size distribution requirements [25].

Standard 1200 × 600 × 6.9 mm^3 SC were manufactured at Calyxo from the test powder batch at different thin film sputter deposition process parameters following a unique patented technology [26]. The electrical parameters of the test SC showed compliance with the industrial CX3 power output standard [26], some test SC parameters being even superior to the standard ones. Table 1 presents some electrical parameters of the test SC.

However, endurance tests conducted following the manufacturer's method [26] showed that the test SCs undergo faster degradation than standard ones.

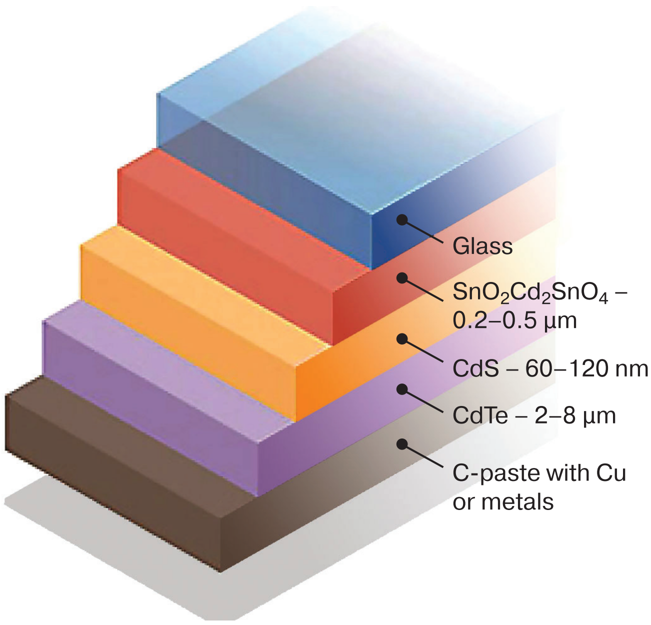

Figure 1. Typical CdTe SC structure [9]

Table 1. Comparison between some electrical parameters of test solar cells and CX3 Grade cadmium telluride thin-film solar cells

Electrical parameter	Solar cell	
	Test specimen	CX3
Rated power output P_{mpp} (W)	87.0	85.0
Short circuit current I_{sc} (A)	2.2	2.0
Open circuit voltage V_{oc} (V)	60.5	62.0

In order to understand the origin of the unstable properties exhibited by the test SC during the endurance tests we studied the powders and the films made from them at the Joint Use Center of the National University of Science and Technology MISIS. The test materials were CdTe powders, purity at least 5N (99.999 wt.%) synthesized by ADV. The reference specimens were powders used by Calyxo for their manufacture having the same grain size distribution ranging from 125 to 250 mm. Furthermore we studied the surface structure of the films made from these powders by Calyxo at standard SC process parameters, before and after endurance tests.

The phase composition of the materials was studied by X-ray diffraction on a Bruker AXS D8 Discover diffractometer. The structure and elemental composition of the specimens were studied under a JEOL JSM-6480LV scanning electron microscope (SEM) with an Oxford Instruments INCADRYCOOL energy dispersion attachment.

3. Results and discussion

Study of the phase composition and crystalline structure parameters of the specimens showed that the powder synthesized by ADV contains along with the CdTe phase a very small quantity of excess tellurium (trace amount close to the method's resolution). The powder made by Calyxo and the films made from it are single-phase according to X-ray diffraction data, the lattice parameter of CdTe in the film not changing after endurance tests. The films made from the ADV powder did not contain excess tellurium but the CdTe phase lattice parameter changed after endurance tests unlike for the films made from Calyxo's standard powder. In our opinion this is caused by the excess tellurium in ADV's powder which is present in the form of an amorphous phase localized at the grain boundaries in the film. Data on the phase composition of the CdTe specimens are summarized in Table 2.

Secondary electron SEM studies of the CdTe thin films made from Calyxo's and ADV's powders did not reveal any difference before and after the endurance tests. The coatings are continuous and uniform, without pores or

Table 2. Phase composition and lattice parameters of cadmium telluride specimens

Specimen	Phase composition	Concentration (vol.%)	Lattice parameter (nm)
Calyxo powder	CdTe	100	a = 0.6483
ADV powder	CdTe	96	a = 0.6483 a = 0.4457 c = 0.5929
	Te	4	
Calyxo films before endurance tests	CdTe	100	0.6492
ADV films before endurance tests	CdTe	100	0.6490
Calyxo films after endurance tests	CdTe	100	0.6492
ADV films after endurance tests	CdTe	100	

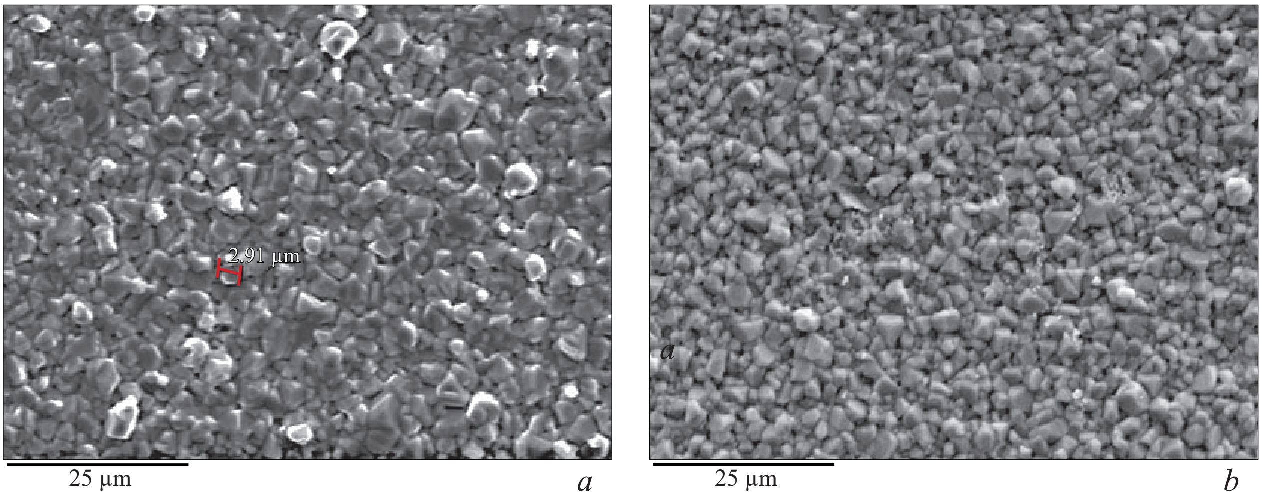

Figure 2. SEM morphology of films made from Calyxo powders (*a*) before and (*b*) after endurance tests

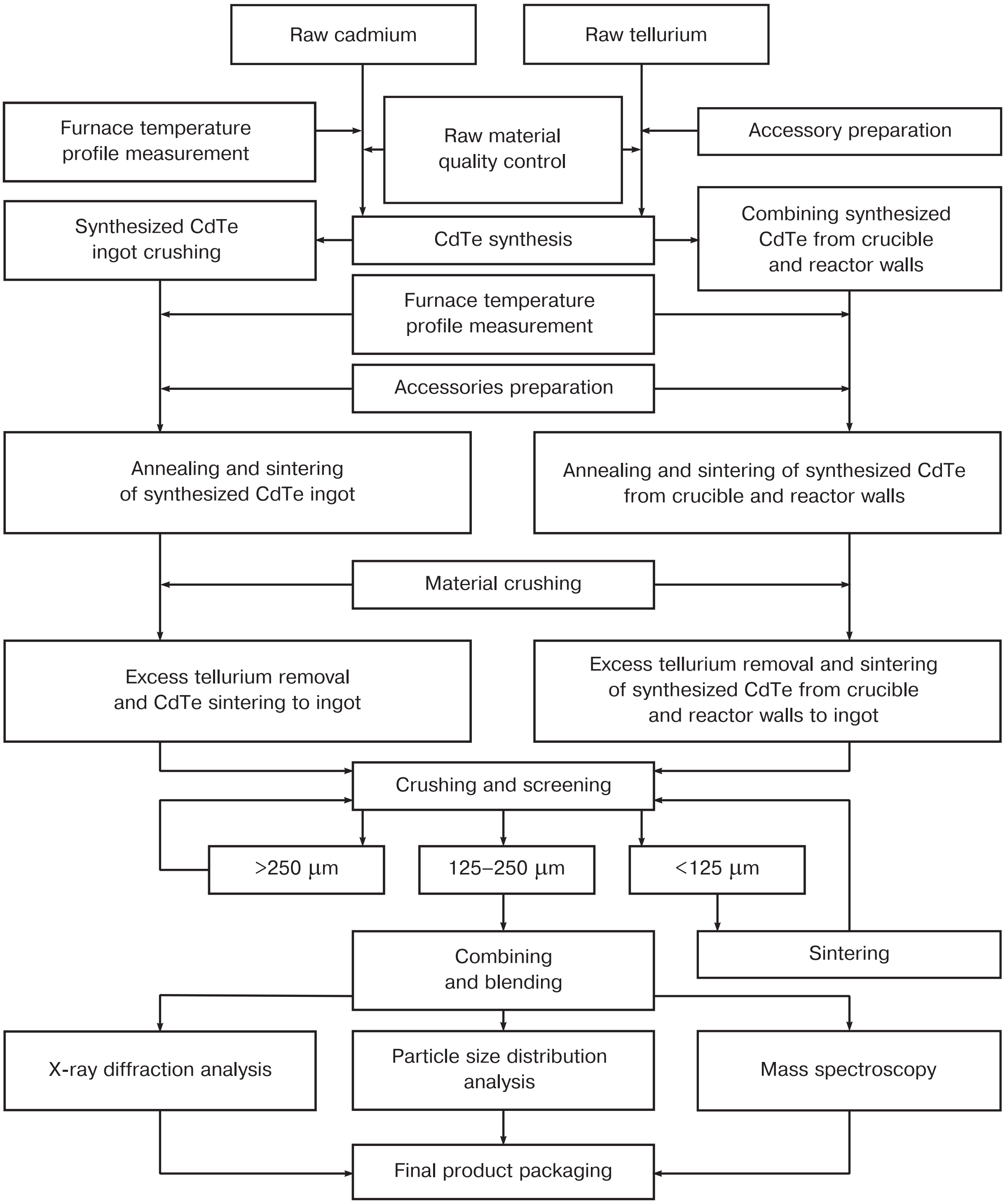

Figure 3. CdTe powder process route providing required properties and grain size distribution

cracks, the grain size ranging from 1 to 5 mm. The structure and morphology of the films did not change after the endurance tests.

The elemental composition of the films at different points was the same before and after the endurance tests within the accuracy of the energy dispersion X-ray spectroscopy method. No free tellurium was found in the ADV specimens since its content was below the method's resolution and possibly because it was predominantly localized at the grain boundaries.

Figure 2 shows example of SEM film morphology for the films made from Calyxo's powder before and after the endurance tests.

In order to eliminate the abovementioned disadvantages we significantly improved the currently used CdTe powder technology. A new direct synthesis process route for CdTe powder in a quasi-air-tight quartz reactor was developed, proven and tested (Fig. 3) taking into account the advantages and drawbacks of the existing technology.

Furthermore, process accessories and parameters were improved for some process stages.

The process route can be divided into four stages.

1. Preparation of main and auxiliary materials, process accessories and equipment for the main processes. This stage includes the following processes:

– chemomechanical preprocessing of the main materials used in the synthesis process including, where necessary, crushing of the raw materials by grinding;

– chemomechanical preprocessing and annealing of quartz and graphite accessories used at the main process stages;

– temperature field (profile) measurements at the furnace units of the process equipment;

– condition control, maintenance and repair of the main and auxiliary process equipment.

2. CdTe synthesis, special annealing and sintering of high-quality material having the required stoichiometriuc composition. This stage includes the following processes:

- CdTe direct synthesis in a quasi-air-tight quartz reactor;

– synthesized material separation into CdTe ingots and CdTe from crucible and reactor walls;

– special annealing (using special equipment and accessories) and separate sintering of the CdTe ingots and CdTe from crucible and reactor walls for the production of CdTe having the required stoichiometriuc composition;

– sintering of CdTe fine fractions.

3. Crushing of the materials produced at the previous process stages to powder having the required grain size distribution (grinding and screening), powder combining and blending. This stage includes the following processes:

– crushing of the materials produced as a result of the synthesis and sintering stages on a jaw crusher and a disc mill pulveriser;

– crushing and grinding on an disc mill pulveriser followed by material screening into customer-specified size fractions with calibration screens on a vibration table;

– material composition blending by mixing in a tumbling drum.

4. Interim and final material quality control including the following control operations:

– control of raw materials and final products for elemental composition using mass spectroscopy and atomic emission (where required) methods;

– control of final product grain size distribution by particle size distribution analysis;

– control of final product phase composition and stoichiometry using X-ray diffraction.

At the first phase of new process route test run, every process stage was followed by a study of the phase and elemental composition of the synthesized materials. The phase composition of the materials was studied using the method as described above and the elemental composition was studied at the Test Analytical and Certification Center of Giredmet JSC using spark mass spectroscopy on a JEOL JMS-01-BM2 double focus instrument (Japan).

Experiments following the above described schedule confirmed the correctness of the new technical solutions chosen: the materials had a purity of not worse than 5N (for the main material CdTe) and no excess tellurium or cadmium phases were found in the CdTe powder.

4. Conclusion

A batch of CdTe material having the preset purity and grain size distribution was produced using direct synthesis method. Test SCs having parameters compliant with worldwide standards were manufactured from the test powder batch using a unique technology and subjected to endurance tests.

The effect of free tellurium phase in the powder on the endurance of the devices made from the powder was studied by comparing the properties of the CdTe powders synthesized in this work and the films made from the powders. We show that if a second phase is present in the CdTe films the excess tellurium is predominantly localized at the grain boundaries and can change the electrical properties of the product SC in the course of failure-free operation. Excess tellurium changes the lattice parameters of the CdTe phase in the films due to a change in the stoichiometric composition of the CdTe phase. Thin film specimens were also studied using secondary electron scanning electron microscopy. The SEM study did not reveal any differences before and after endurance tests, the coatings were continuous and uniform, without pores or cracks, the grain size ranging from 1 to 5 mm. The structure and morphology of the films did not change after the endurance tests.

A new cadmium telluride powder process route was developed, proven and tested taking into account the advantages and drawbacks of the previously used process. Experiments confirming the correctness of the technical solutions chosen were conducted. Powders with a purity of not worse than 5N (for the main material CdTe) were synthesized and proved to contain no excess tellurium or cadmium phases.

The main advantage of the newly developed process are relatively simple process equipment required coupled with a high yield of high-quality final product, as well as process scalability greatly contributing to a competitive product cost and hence a reduction of SC price per 1 W.

Further work in this field will include the fabrication of test SCs from the CdTe powders synthesized using the new process and studies of their properties.

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