



ON LEAD POWDER ELEMENTARY CELL PROPERTIES VARIATION UNDER CRYOGENIC CONDITIONS

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Abstract: Lead is a very important metallic material because of its using in anti radiation shields and in ecological recharging batteries. This purpose of this article is the investigation of the lead elementary cell properties under cryogenic conditions. The X-ray diffraction analysis performed at low temperatures proves that crystal parameter decreases linearly with temperature which implies a linear variation of volume and density of elementary cell. The volume presents a strong decreasing with temperature meanwhile density is proportional increased. The increasing of density directly proportional with temperature decreasing makes lead suitable as anti radiation shield under cryogenic conditions. There were calculated the values of lead elementary cell: crystal parameter 492.46 pm, elementary cell volume 119.43 pm³, and the density of 11.524 g/cm³ at 0K.

Key words: lead powder, low temperature, elementary cell.

1. INTRODUCTION

Lead is a very important metallic material with applications in a wide range of industrial branches. It is regarded as only material which offer full protection against radiation electromagnetic sources as well as gamma radiations [1 – 3]. Some researches were developed to achieve composite shields alternating lead and polymer sheets [4, 5].

Lead is involved into another major application in recharging batteries. A Pb – Li electrode is used in order to eliminate the using of cadmium and mercury [6 – 8]. This provides more ecological recharging batteries.

The applications mention above, are suitable in cryogenic conditions. Several studies achieve significant information related to the thermal expansion coefficient variation [9 – 11]. In some cases there could be reach out some other interesting material properties related to the particularly crystal lattice. Crystal structure of lead allows the determination of crystal cell properties from the X-ray diffraction data [12, 13]. The main goal of present research is to investigate the elementary cell properties for lead powder at different cryogenic temperature and to observe their variation.

2. THEORETICAL TREATMENT

The X-ray diffraction investigation is able to reveal the crystalline state of the lead powder, respectively allows the deduction of the crystal structure [12, 13]. The basic value measured by X-ray diffraction is the interplanar distance of diffracting planes described by Bragg's Law:

$$\frac{d}{n} = \frac{\lambda}{2 \sin \theta}, \quad (1)$$

where: d – interplanar distance, n – diffraction order n = 1 for monochrome wavelength, λ – X-ray wavelength, and θ – the Bragg diffraction angle.

Lead crystallizes in FCC crystal system [9, 10]. Considering the crystallographic relations for FCC lattice the crystal parameter a_i is expressed:

$$a_i = d \cdot \sqrt{h^2 + k^2 + l^2}, \quad (2)$$

where: h, k, and l are Miller indices of the diffractant plane.

Furthermore the lattice parameter could be calculated by the least square method:

$$a_i = a_0 + bf.$$

(3)

where: a_0 – extrapolated lattice parameter at $2\theta = 180^\circ$, a_i – resulted lattice parameter for each diffraction peak, f – extrapolation function [9]:

$$f = \frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta}. \quad (4)$$

The elementary cell properties could be calculated using the a_0 value of crystal parameter related to the lead atom properties. The elementary cell density is described by following equation:

$$\rho = m / V \quad (5)$$

where: m – mass, and V – volume. The elementary cell mass is expressed:

$$m = N \cdot \frac{A_{Pb}}{N_A}, \quad (6)$$

where: N - number of atoms, A_{Pb} – atomic mass of lead, N_A – the Avogadro Number. Finally the volume of elementary cell is given by:

$$V = a_0^3. \quad (7)$$

The presented relations allow us to calculate with high accuracy the mentioned properties of lead elementary cell. It is interesting to observe the behavior of these properties under different cryogenic temperatures.

3. RESULTS AND DISCUSSION

The X-ray diffraction investigation was performed on a DRON 3 X-ray diffractometer equipped with data acquisition module and Matmec VI.0 soft. All X-ray diffraction patterns were obtained with $Cu_{K\alpha}$ radiation. The cryogenic investigation was performed with special device UNRT 180 coupled on the DRON 3 diffractometer with liquid nitrogen cooling. Lead powder sample was investigated at several low temperatures (298, 273, 223, 173, and 123 K). The total exposure time of each

sample at cryogenic temperatures is 55 minutes. The resulted X-ray patterns are presented in Figure1.

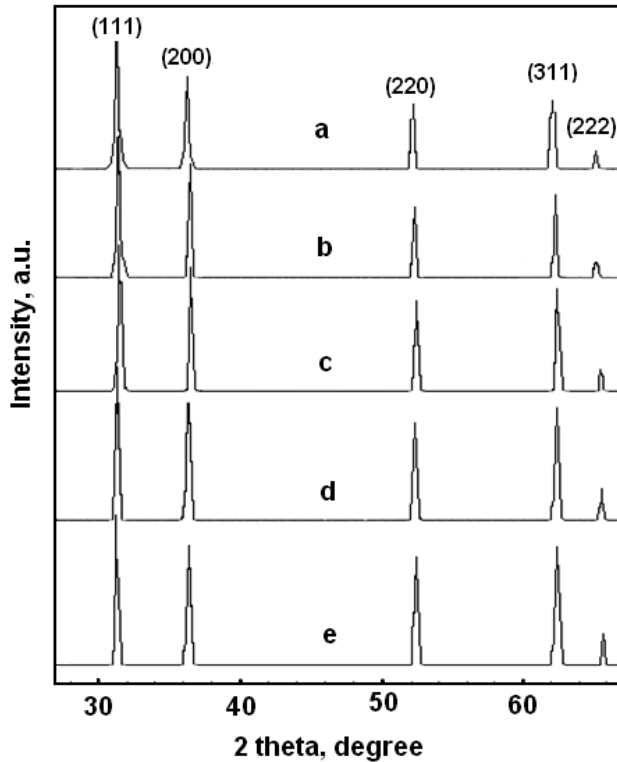


Fig. 1. The X-ray diffraction spectra for lead powder at different temperatures: a) 298 K, b) 273 K, c) 223 K, d) 173 K, and e) 123 K. Figures in brackets are Miller indices.

The X-ray pattern resulted at room temperature (298 K) presents well developed peaks corresponding to an annealed state of lead powder, Figure 1a. Also, a slightly broadening of the diffraction peaks is observed due to the micro scaled powder particles.

A relative increasing of diffraction peaks is observed by decreasing of temperature. The (222) peak present a significant increasing of relative intensity only by a decreasing of temperature to 273 K, Figure 1b.

The observed situation is more pronounced at cryogenic temperatures (223 – 123 K) where (111) and (222) peaks feature a significant increasing of relative intensity related to a reduction of full width at half height (FWHM) comparing to initial state, Figures 1c – 1e. The observed behavior is similar to other alloys such ledeburitic stainless steels [14].

For each X-ray diffraction pattern in Figure 1 were determined the diffraction angles 2θ and

the interplanar distance was calculated by equation (1). The crystal parameter for each diffraction peak, a_i , was calculated using equation (2). The crystal parameter a_0 was calculated according to relations (3) and (4). Finally, the crystal parameter versus temperature is presented in Figure 2.

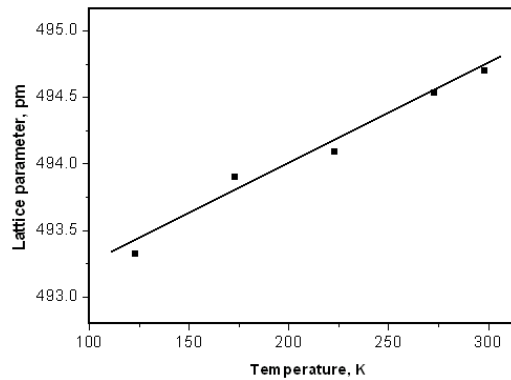


Fig. 2. Lattice parameter versus temperature.

The temperature decreasing conducts to a severe shrinkage of crystal lattice observed by the decreasing of crystal parameter. The variation in Figure 2 presents a linear trend which allows the calculation the absolute value of crystal parameter at 0 K. The resulted value of absolute crystal parameter is 492.46 pm.

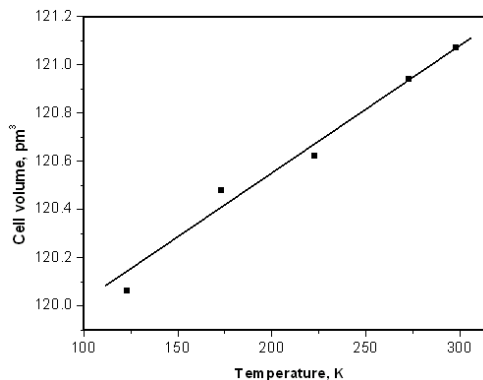


Fig. 3. Elementary cell volume versus temperature.

The crystal parameter gives directly the influence on variation of elementary cell volume, Figure 3. It value was calculated for each temperature with equation (7). The resulted value of elementary cell volume is 1194.43 pm^3 at 0 K.

The decreasing of the elementary cell parameter and volume with temperature decreasing induces a significant approach of the lead atoms in crystal lattice. The atom approach related to the volume reduction cause a significant increasing of density. The density of

elementary cell was calculated for each temperature using equations (5 – 7).

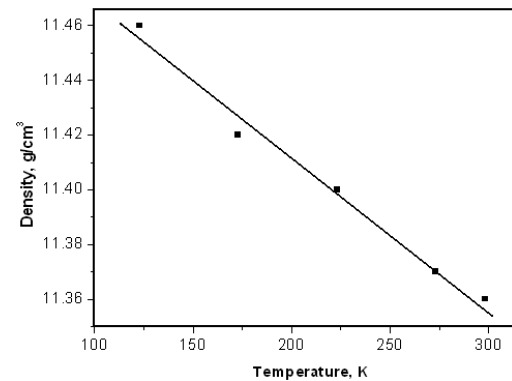


Fig. 4. Density versus temperature.

The density variation with temperature is presented in Figure 4. There is observed the severe increasing of density in the cryogenic range. The value of lead elementary cell density is 11.524 g/cm^3 at 0 K, significant increased than the density at room temperature (11.4 g/cm^3 [12]). The increased density of the lead elementary cell indicates that lead is suitable for anti radiation shield in cryogenic conditions.

4. CONCLUSIONS

The X-ray diffraction analysis performed at low temperatures proves that crystal parameter decreases linearly with temperature which implies a linear variation of volume and density of elementary cell. The volume presents a strong decreasing with temperature meanwhile density is proportional increased. The increasing of density directly proportional with temperature decreasing makes lead suitable as anti radiation shield under cryogenic conditions. There were calculated the values of lead elementary cell: crystal parameter 492.46 pm, elementary cell volume 1194.43 pm^3 , and the density of 11.524 g/cm^3 at 0 K.

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Asupra variației proprietăților celulei elementare a pulberii de plumb în condiții criogenice

Rezumat: *Plumbul este un material metalic foarte important atât din punct de vedere al protecției antiradiații cât și pentru utilizarea la bateriile reîncărcabile ecologice. Prezentul articol are ca scop investigarea proprietăților celulei elementare în condiții criogenice. Analizele de difracție cu raze X efectuate la temperaturi joase arată că parametrul cristalografic al plumbului prezintă o scădere liniară direct proporțională cu scăderea temperaturii. Faptul conduce la o scădere corespunzătoare a volumului celulei elementare concomitent cu o creștere a densității acestuia. Creșterea densității plumbului proporțional cu scăderea temperaturii arată că acesta se pretează ca scut antiradiații la temperaturi criogenice. Au fost calculate valorile absolute caracteristice pentru celula elementară a plumbului: parametrul cristalografic 492,46 pm; volumul celulei elementare 119,43 pm și densitatea acesteia 11,524 g/cm³.*

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