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The quest for direct band beta iron disilicide: collaboration of theoretical and experimental approaches

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Abstract. In the presented work, a theoretical study of the effect of β-$FeSi_2$ lattice deformation on the type and magnitude of the first transition in the electronic band structure was carried out. Images of nanocrystallites obtained using high-resolution transmission electron microscopy were used as a source of deformation data. All in all, 137 variants of β-$FeSi_2$ lattice deformation were considered in the work. Six types of first transitions different from the first transition in unstrained β-$FeSi_2$ were discovered. The values of the first transitions from 0.02 to 0.64 eV (direct) and from 0.01 to 1.12 eV (indirect) were obtained.

Keywords: silicon, beta Fe disilicide, *ab initio* calculation

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Поиски прямозонного бета-дисилицида железа: взаимодействие теоретических и экспериментальных подходов

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Аннотация. В представленной работе было проведено теоретические исследование влияния деформации решетки β-$FeSi_2$ на тип и величину первого перехода в электронной зонной структуре. В качестве источника данных о деформации использовались изображения нанокристаллитов, полученных с помощью просвечивающей электронной микроскопии высокого разрешения. Всего в работе рассмотрено 137 вариантов деформации решетки β-$FeSi_2$. Обнаружено 6 типов первых переходов, отличающихся от первого перехода в недеформированном β-$FeSi_2$. Получены величины первых переходов от 0.02 до 0.64 эВ (прямые) и от 0.01 до 1.12 эВ (непрямые).

Ключевые слова: кремний, бета дисилицид Fe, первопринципные расчеты

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Introduction

In accordance with modern investigations β-$FeSi_2$ can be applied in light emitting, light absorbing and thermoelectric devices [1–5]. In all of these cases, it is significant to understand electron band structure nature of the material. Previous studies have shown that β-$FeSi_2$ light emitting ability depends on change of the fundamental transition as a consequence of lattice deformation. Lattice parameter variation is especially pronounced, when nanocrystallites (NCs) are embedded under different conditions. Within this investigation a wide range of high-resolution transmission electron microscopy (HRTEM) data was analyzed to extract information about β-$FeSi_2$ lattice deformation embedded into Si under different conditions. Based on the data obtained, *ab initio* calculations were carried out and the results will be discussed below.

Calculation details

The density-functional theory calculations were performed with the package VASP [6]. The plane-wave basis with the ultra-soft Vanderbilt pseudopotential [7] and the generalized gradient approximation (GGA) to the exchange-correlation functional were used. Non-spherical contributions from the gradient corrections were included. Monkhorst–Pack *k*-points grid [8] of 8×8×8 was used. The cut-off energy was of 350 eV. Relaxation was performed with respect to the atoms' positions, volume, and the shape of the cell. The obtained lattice constants were $a = 9.907$ Å, $b = 7.781$ Å, and $c = 7.833$ Å (experimental values are $a = 9.863$ Å, $b = 7.791$ Å, and $c = 7.833$ Å [9]). The indirect fundamental energy gap was found of 0.60 eV (the GGA theoretical value of Ref. [10] is 0.62 eV and the experimental value is 0.839 eV [11]).

Results and Discussion

HRTEM data of one sample was analyzed to obtain NCs sizes and lattice deformation value. Fig. 1, *a* shows broad NCs size distribution. For theoretical investigation bulk β-$FeSi_2$ cell was deformed in accordance with NCs deformation: 14 NCs in diameter range from 3.5 nm to 10 nm were considered. Calculation results are shown in (Fig 1, *b*, *c*). The first conclusion is even within one sample NCs with different first transition type can be observed. The second one is NC size is related to the first transition type, but this is not a determining factor, since there is a wide NC diameters range, where both direct and indirect first transition types coexist. The third one is general lattice strain expressed as a change in cell volume as well is not a determining factor for similar reason.

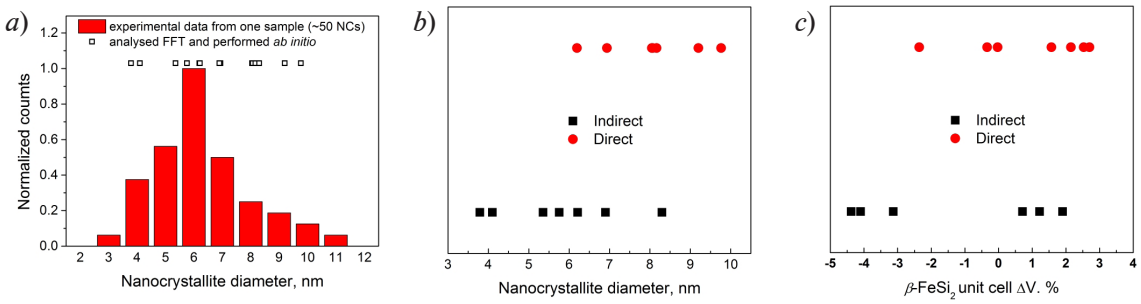

Fig. 1. Distribution of β-$FeSi_2$ nanocrystallite diameter within one sample (*a*) and calculated first transition type: depending on nanocrystallite diameter (*b*), depending on unit cell volume change (*c*)

The next step was to check how β-$FeSi_2$ band structure changes with a particular deformation with a significant data collection. HRTEM data were collected from literature and our previous experiments. All in all, 137 NCs were analyzed within this work to determine lattice deformation and then electron band structure was calculated for each strained cell. 113 of them had indirect type band gap and 24 ones had direct type band gap. Structures with direct band gap type are in deformations range of Δa from +0.6 to +7.3%, Δb from −8.1 to +6.2%, Δc from −4.1 to +1.8%. Structures with indirect band gap types are in deformations range of Δa from −9.7 to +10.4%, Δb from −6.0 to +7.3%, Δc from −7.7 to +5.3% as shown in Fig. 2. Positive Δ value corresponds to tension and negative one corresponds to compression. Thus β-$FeSi_2$ has narrow range of a and c lattice constants deformation, which allow existence of band structure with the first transition of direct type. On the other hand, β-$FeSi_2$ shows flexible band structure depending on deformation allowing to obtain band gap in range from 0.02 to 0.64 eV (direct type) and in range from 0.01 to 1.12 eV (indirect type), that is opportunity to create light emitting and receiving devices of different frequency ranges using different creation conditions, but same material.

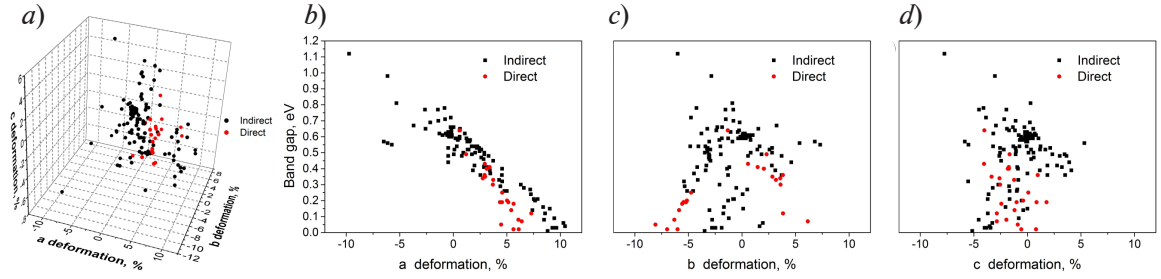

Fig. 2. First transition type in β-$FeSi_2$ depending on deformation: 3D plot of transition type (*a*) and band gap value depending on the deformation: lattice parameter *a* (*b*), lattice parameter *b* (*c*), lattice parameter *c* (*d*). Positive deformation corresponds to tension and negative one corresponds to compression. Points on *a* plot correspond to ones on *b*–*d*. Band gap axis on *b* plot is common for *b*–*d* ones

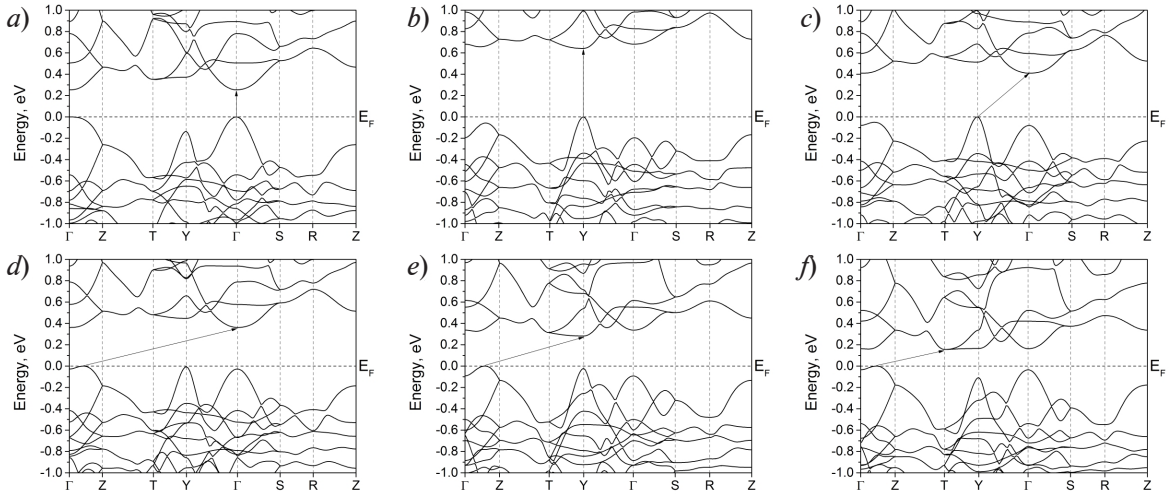

Fig. 3. Electron band structure in β-$FeSi_2$ depending on the deformation (Δa, Δb and Δc are specified for each plot): +4.6%, -4.8%, +0.1% (*a*), +0.6%, -1.3%, -4.0% (*b*), +2.9%, -1.2%, +3.2% (*c*), +4.5%, -1.3%, +1.9% (*d*), +6.6%, -0.5%, -3.2% (*e*), +8.4%, 1.7%, -2.0% (*f*)
The Fermi level is taken as the zero-energy point. Arrows show the first transition

The other side of β-$FeSi_2$ band structure flexibility is location of the first transitions in reciprocal space. Fig. 3 shows obtained band structures with examples of fundamentally different first transitions: 2 direct (Γ→Γ, Y→Y) and 4 indirect ones (Y→Γ, Λ*→Γ, Λ*→Y, Λ*→T). Unstrained bulk β-$FeSi_2$ has Y→Λ* first transition. On the one hand direct-indirect type change is a reason

why light radiation can be observed from some NCs, but not from others of similar size, on the other hand different direct transition positions in reciprocal space explain different experimentally observed luminescence spectra: band walleyes located in various points have various charge carrier effective mass, oscillator strength and energy with regard to Fermi level.

Conclusion

It was demonstrated that within one sample β-$FeSi_2$ NCs with both direct and indirect first transition type can coexist. Neither NC diameter nor cell volume change are not a factor determining the first transition types. There was shown that the first transition of direct type exists in narrow deformation range of 7.9%, 14.3% and 5.9% for a, b and c lattice constants, respectively. Whereas indirect one exists in wide range of 20.1%, 13.3% and 13.0% for a, b and c lattice constants, respectively. Six first transition types differed from fully relaxed bulk β-$FeSi_2$ were observed: 2 direct (Γ→Γ, Y→Y) and 4 indirect ones (Y→Γ, Λ*→Γ, Λ*→Y, Λ*→T).

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