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Thermal and electrical conductivity of grain boundaries in metals with bcc and fcc crystal lattices

E.V. Morozova [1] ✉, D.A. Timkaeva [1]

[1] Ulyanovsk State University, Ulyanovsk, Russia

✉ kat-valezhanina@yandex.ru

Abstract. This study employs first-principles calculation methods to investigate the thermoelectric properties of high-angle grain boundaries in metals (iron, titanium, copper, and nickel) with symmetric tilt boundaries of two types of crystal lattice: body-centered cubic and face-centered cubic. Grain boundaries play a significant role in carrier and phonon transport in materials. Altering geometric parameters is one of the simplest ways to control thermoelectric characteristics. By varying the grain rotation axis, rotation angle, and grain self-orientation, we derived the dependence of the electrical and thermal conductivity of studied materials on the geometry of the modeled device at room temperature. The results presented in the work can give an idea of the effect of this type of surface defect on thermal and electrical conductivity.

Keywords: grain boundary, electrical conductivity, thermal conductivity

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Тепло- и электропроводность границ зерен в металлах с ОЦК и ГЦК кристаллическими решетками

Е.В. Морозова [1] ✉, Д.А. Тимкаева [1]

[1] Ульяновский государственный университет, г. Ульяновск, Россия

✉ kat-valezhanina@yandex.ru

Аннотация. В данной работе использованы первопринципные методы расчета для исследования переноса электронов и фононов в высокоугловых границах зерен металлов (железо, титан, медь и никель) с симметричным наклоном границы двух типов кристаллической решетки: объемоцентрированная и гранецентрированная кубическая. Варьируя ось вращения зерен, угол поворота и собственную ориентацию зерен, мы получили зависимость транспорта электронов и фононов от геометрии моделируемого устройства. Результаты, приведенные в работе, могут дать представление о влиянии такого типа поверхностного дефекта на тепло- и электропроводность.

Ключевые слова: граница зерна, электрическая проводимость, теплопроводность

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Introduction

The grain boundary (GB) is a two-dimensional (surface) defect in the atomic structure, separating two differently oriented grains (crystallites). Typically, it is a disordered multi-atom system with a wide variety of forms. GBs play a significant role in carrier and phonon transport in materials [1–2]. Various studies indicate that GBs are an active element of the material's defect structure, affecting properties such as plasticity, diffusion, fracture, and deformation at elevated temperatures, among others. The bonding at GBs differs from that in a regular crystalline lattice. Due to the formation of a specific structure at the grain contact region different from the perfect crystal structure, the properties of boundaries can differ from those of the bulk material [3–7].

At low temperatures, the resistivity of metals depends on the scattering of electrons on defects in the crystal lattice, and the contribution of thermal vibrations of lattice atoms should tend to zero. Metals are good conductors of electricity. Typically, such materials are also good heat conductors. In this regard, we will consider the electrical conductivity and thermal conductivity of nano-sized metallic materials with a defect in the form of a grain boundary.

The present study investigates the influence of a surface defect such as GB on the thermoelectric properties of grains of transition metals (iron, copper, titanium, nickel) and semiconductors (silicon carbide, boron nitride) with face-centered cubic and body-centered cubic lattices.

Materials and Methods

The calculations were carried out within the framework of the Slater-Koster method using the Density Functional Based Tight Binding (DFTB) formalism for electronic properties and molecular dynamics for thermal characteristics. The system, simulating the device, was divided into three regions: the left and right semi-infinite electrode regions and the central part. Transport coefficients were calculated using the non-equilibrium Green's function (NEGF) method, density functional theory (DFT), and non-equilibrium molecular dynamics. The studied parameters were computed using the following relationships:

$$G_{\mathrm{e}} = \left.\frac{dI}{dV_{\mathrm{bias}}}\right|_{dT=0}, \quad S = -\left.\frac{dV_{\mathrm{bias}}}{dT}\right|_{I=0}, \quad \lambda_{\mathrm{e}} = \left.\frac{dI_Q}{dT}\right|_{I=0}, \quad \Pi = \left.\frac{I_Q}{I}\right|_{dT=0} = SV_{\mathrm{bias}}. \tag{1}$$

Here, S is the Seebeck coefficient, G_{e} is electrical conductivity, T is absolute temperature, λ is thermal conductivity, which is equal to the sum of electronic λ_{e} and phonon λ_{ph} thermal conductivity, $I_Q = \mathrm{d}Q/\mathrm{d}T$ is the electronic component of the heat flux.

Results and Discussion

In our work, to obtain the dependences of electrical and thermal conductivity, we changed such geometric parameters of symmetrical grain boundaries as the rotation axis of the grains, the rotation angle, and the proper orientation of the grain boundary in space. Structure parameters are indicated in the Table. Examples of the calculation results are presented in Figures 1 and 2.

Near the Fermi level, the maximum thermal conductivity of nickel is greater than that of copper by 1.7. A similar relationship is observed for electrical conductivity.

The maximum conductivity of iron is achieved at grain rotation axes [001] and exceeds the minimum conductivity of 1.4 near the Fermi level.

Table

Characteristics of symmetrical inclined grain boundaries of metals

Axis of rotation	Name sample	Grain boundary	Disorientation angle	Lattice type
[001]	Fe	Σ 5(–2–10)	53.13°	bcc
[011]	Fe	Σ 3(11–1)	70.53°	bcc
[111]	Fe	Σ 3(–12–1)	60°	bcc
[111]	Ti	Σ 3(–12–1)	60°	bcc
[111]	Cu	Σ 3(–12–1)	60°	fcc
[111]	Ni	Σ 3(–12–1)	60°	fcc

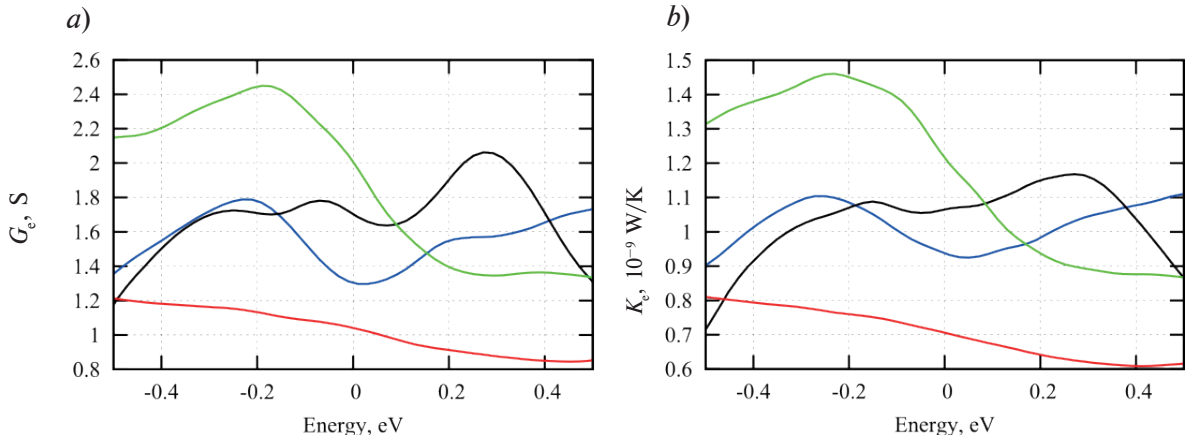

Fig. 1. Electrical conductivity (*a*) and thermal conductivity (*b*) coefficients for symmetric grain boundaries in metals with a [111] rotation axis: Fe – blue curve, Ti – black curve, Cu – red curve, Ni – green curve

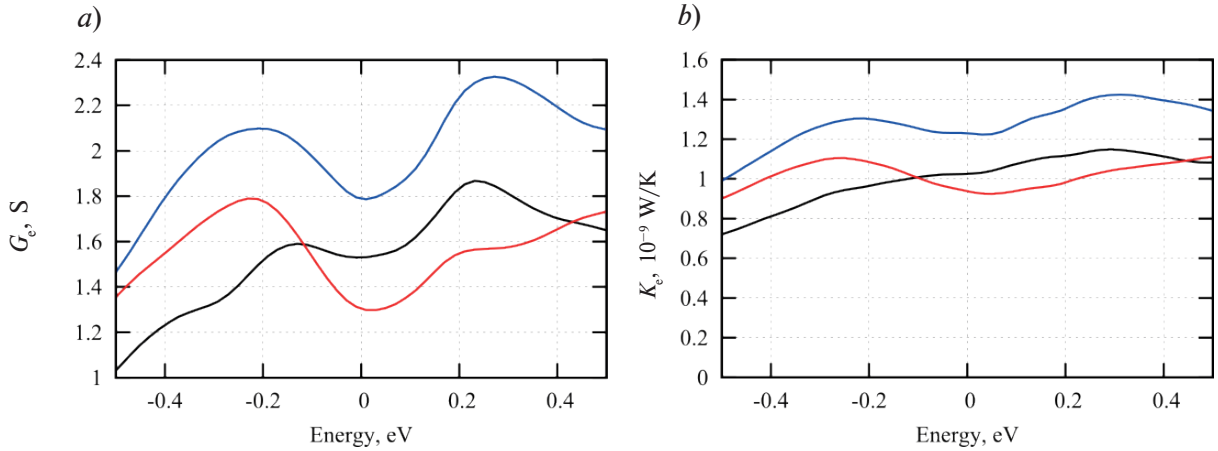

Fig. 2. Electrical conductivity (*a*) and thermal conductivity (*b*) coefficients for the symmetric grain boundary of iron with rotation axes [001] (blue curve), [011] (red curve), and [111] (black curve) are provided

Conclusion

Based on the results obtained, it can be concluded that the grain rotation axis and misorientation angle affect the conductivity parameters of the device to varying degrees for each material. For instance, metals with a face-centered cubic lattice will exhibit the highest electrical conductivity coefficient with grain rotation axes [001] and [011].

Contrary to the statement that highly conductive materials should conduct heat well, in low-dimensional metal structures, namely iron, titanium, nickel and copper, we observe low thermal conductivity (on the order of 0.7 to 2 nW/K) with comparatively high electrical conductivity (up to 2 Ohm^{-1} units). Then concludes that the grain boundary defect in metals can be used in nanostructured materials for thermal insulation applications.

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THE AUTHORS

MOROZOVA Ekaterina V.
kat-valezhanina@yandex.ru
ORCID: 0000-0002-7530-3933

TIMKAEVA Diana A.
dianatimkaeva@mail.ru
ORCID: 0000-0003-3748-0696

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