Mixed Mismatch Model for Predicting Metal/Semiconductor Interface Thermal Conductance

Authors: Zong Zhicheng, Pan Dongkai, Deng Shichen, Wan Xiao, Yang Lina, Ma Dengke, Yang Nuo, Yang Nuo

Date: 2022-10-17T00:00:00+00:00

Abstract

The acoustic mismatch model and diffuse mismatch model are widely applied in the calculation of interface thermal conductance, with the two models being established upon assumptions of extremely smooth and rough interfaces, respectively. Owing to considerable discrepancies between actual interface structures and these two assumptions, the predicted results from both models deviate significantly from the actual interface thermal conductance. A recently proposed hybrid mismatch model accounts for the influence of interface structure on the proportion of specular phonon transmission and diffuse transmission, thereby achieving enhanced prediction accuracy. However, this model necessitates complex molecular dynamics simulations to acquire interfacial phonon information. Consequently, this study simplifies the hybrid mismatch model by incorporating measured roughness values and further considers the impact of interface structure on contact area, thereby enabling simple, rapid, and accurate prediction of interface thermal conductance. Utilizing this model, this work calculates and predicts the interface thermal conductance between metals (aluminum, copper, gold) and semiconductors (silicon, silicon carbide, gallium arsenide, gallium nitride). The results for the aluminum/silicon interface are compared with experimental measurements, demonstrating favorable agreement. This model not only contributes to the understanding of interfacial thermal conduction mechanisms but also facilitates comparison with experimental results.

Full Text

Mixed Mismatch Model for Predicting Interfacial Thermal Conductance at Metal/Semiconductor Interfaces

Zong Zhicheng[1]), Pan Dongkai[1]), Deng Shichen[1]), Wan Xiao[1]), Yang Lina[2]), Ma Dengke[3]), Yang Nuo[1])†

[1]) School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan 430074, China
[2]) School of Aerospace Engineering, Beijing Institute of Technology, Beijing 100081, China
[3]) School of Physics and Technology, Nanjing Normal University, Nanjing 210000, China

Abstract

The acoustic mismatch model (AMM) and diffuse mismatch model (DMM) are widely used for calculating interfacial thermal conductance. These two models are based on the assumptions of perfectly smooth and completely rough interfaces, respectively. However, actual interface structures differ significantly from these idealized conditions, leading to substantial deviations between model predictions and measured interfacial thermal conductance. The recently proposed mixed mismatch model (MMM) improves prediction accuracy by considering how interface structure affects the ratio of phonon specular transmission to diffuse scattering. Nevertheless, this model requires complex molecular dynamics simulations to obtain interfacial phonon information, limiting its broader application. To address this limitation, we simplify the MMM by incorporating experimentally measured roughness values and additionally account for the effect of interface structure on contact area, enabling simple, rapid, and accurate prediction of interfacial thermal conductance. Using this simplified model, we calculate and predict the interfacial thermal conductance between metals (aluminum, copper, gold) and semiconductors (silicon, silicon carbide, gallium arsenide, gallium nitride). The predicted results for Al/Si interfaces show good agreement with experimental measurements. This model not only facilitates understanding of interfacial heat conduction mechanisms but also enables straightforward comparison with experimental data.

Keywords: interfacial thermal conductance, interfacial thermal resistance, metal/semiconductor interface, acoustic mismatch model, diffuse mismatch model
PACS: 63.20.D-, 63.20.kg, 68.35.-p, 44.10.+i
† Corresponding author. E-mail: nuo@hust.edu.cn
First author. E-mail: zhicheng@hust.edu.cn

1. Introduction

The continuous miniaturization of modern electronic devices and rapid increase in power density have made thermal dissipation one of the most critical challenges for device performance and reliability [1-5]. Particularly in nanoscale devices and structures containing high-density interface features, characteristic dimensions have shrunk to the order of the mean free path of energy carriers, making atomic-scale interfacial thermal resistance impossible to ignore [6-10]. The demand for higher-frequency and higher-density microelectronic devices

has created an urgent need to enhance interfacial thermal conductance [11,12].

Understanding thermal transport across metal/semiconductor interfaces is essential for both fundamental thermal science and engineering applications such as thermal management in semiconductor devices. In recent years, interfacial thermal transport has become a research hotspot in both academia and industry [13]. Deng et al. [4] used the diffuse mismatch model to predict the interfacial thermal conductance of SiC/SiO_2 and Si/SiO_2 interfaces, with predictions showing excellent agreement with 3-omega experimental measurements. Yang [10] employed molecular dynamics (MD) simulations to investigate thermal transport across Al/Si interfaces, finding that the degree of atomic disorder at the interface significantly affects phonon transport. Subsequently, Yang et al. [7] used non-equilibrium Green's function (NEGF) methods combined with machine learning algorithms to study how interlayer mass distribution affects interfacial thermal conductance in one-dimensional atomic chains, calculating the mass distribution corresponding to extremal interfacial thermal conductance values. Thermal transport at the nanoscale depends strongly on interface structure [13], with experimental studies revealing that interfacial thermal resistance correlates with several factors including roughness [14-17], interface defects [16,18,19], and growth methods [20-22].

As classical theoretical models for interfacial thermal transport, the acoustic mismatch model (AMM) and diffuse mismatch model (DMM) are widely used due to their simplicity and ease of application. However, AMM and DMM are based on assumptions of perfectly smooth and completely rough interfaces, respectively, without considering specific interface structures, resulting in significant deviations between their predictions and actual interfacial thermal conductance. Zhang et al. [23] proposed the mixed mismatch model (MMM), which considers the effect of interface roughness on the ratio of phonon specular transmission to diffuse scattering, thereby improving prediction accuracy. Nevertheless, this model requires MD simulations to obtain interfacial phonon information, and its complexity has limited broader adoption.

In this work, we simplify the mixed mismatch model by utilizing experimentally measured roughness values, enabling more convenient and efficient prediction of interfacial thermal conductance. Additionally, we incorporate the effect of interface structure on contact area. First, we calculate phonon thermal transport parameters for metals (aluminum, copper, gold) and semiconductors (silicon, silicon carbide, gallium arsenide, gallium nitride) using lattice dynamics and first-principles calculations. Subsequently, based on the simplified MMM, we predict the phonon transmittance and interfacial thermal conductance for these metal/semiconductor interfaces. The calculated results for Al/Si interfaces are compared with experimental measurements, validating the accuracy of our approach.

2. Theory and Methods

For metal/semiconductor interfaces, heat carriers include both phonons and electrons [24]. Regarding the contribution of electrons, researchers have conducted numerous studies. For instance, Singh et al. [25] found that electron-phonon coupling contributions to interfacial thermal transport are negligible based on the Bloch-Boltzmann-Peierls formulation. Hamaoui et al. [26] demonstrated through frequency-domain photothermal radiometry that phonons dominate interfacial thermal transport at metal/silicon interfaces above 150 K. Giri et al. [27] showed via time-domain thermoreflectance measurements that electron-phonon scattering at the interface contributes to interfacial thermal conductance only under highly non-equilibrium conditions between electrons and phonons. Consequently, the importance of electron-phonon coupling for solid-solid interfacial thermal conductance remains controversial [28]. Under equilibrium conditions, electronic contributions to interfacial thermal conductance at metal/nonmetal interfaces are generally considered negligible [13]. Therefore, this study considers only phonon contributions to interfacial thermal conductance.

When incident phonons reach a solid-solid interface between materials A and B, the interfacial thermal conductance can be predicted using Landauer theory via Equation (1):

$$G_m = \frac{1}{4}\sum_j \int_0^{\omega_{A,\max}} D_A(\omega) v_j(\omega) \alpha_{A\to B}(\omega) \frac{\partial n(\omega,T)}{\partial T} d\omega$$

where ω is frequency, $\omega_{A,\max}$ is the cutoff frequency from the phonon dispersion relation of material A, D_A is the phonon density of states (DOS), $n(\omega,T)$ is the Bose-Einstein distribution function, v is phonon group velocity, $\alpha_{A\to B}$ is the phonon transmittance coefficient at the interface, and subscript j denotes different phonon modes. According to Equation (1), the theoretical interfacial thermal conductance G_m can be obtained once the phonon thermal transport parameters on both sides of the interface and the phonon transmittance $\alpha_{A\to B}$ are known. In this work, phonon thermal transport parameters are calculated primarily through lattice dynamics and first-principles methods, while interfacial phonon transmittance is computed using theoretical models.

The AMM and DMM models, as classical interfacial phonon transport models, are expressed as follows [29]:

Acoustic Mismatch Model (AMM):

$$\alpha_{A\to B}^{\mathrm{AMM}} = \frac{4\rho_A v_A \rho_B v_B}{(\rho_A v_A + \rho_B v_B)^2}$$

Diffuse Mismatch Model (DMM):

$$\alpha_{A\to B}^{\mathrm{DMM}} = \frac{\sum_j D_B(\omega) v_B(\omega)}{\sum_j D_A(\omega) v_A(\omega) + \sum_j D_B(\omega) v_B(\omega)}$$

The AMM assumes only transmission and reflection at the interface, while DMM assumes completely diffuse scattering. However, at real solid-solid interfaces, phonons simultaneously undergo transmission, reflection, and diffuse scattering [30,31]. Therefore, the MMM introduces a specularity parameter p to represent the fraction of specular phonon transmission at the interface, with the diffuse scattering fraction being $(1-p)$. The phonon transmittance is then defined as a linear combination of AMM and DMM [23]:

$$\alpha_{A\to B}^{\mathrm{MMM}} = p \cdot \alpha_{A\to B}^{\mathrm{AMM}} + (1-p) \cdot \alpha_{A\to B}^{\mathrm{DMM}}$$

Ziman et al. [32] noted that the specularity parameter p depends on the root-mean-square roughness η and phonon wavelength λ, establishing this relationship as:

$$p = \exp\left(-\frac{2\pi^2\eta^2}{\lambda^2}\right)$$

The key to Equation (5) is obtaining the interfacial roughness η. Zhang et al. [23] employed MD simulations of Al/Si interfaces and used DOS to characterize η, but the complex modeling and computational time required for MD make the MMM model difficult to use widely. Therefore, this work substitutes experimentally measured roughness values η from previous researchers into Equation (5) to obtain the specularity parameter p, enabling straightforward application of the MMM model for interfacial thermal conductance calculations and comparison with experimental results.

Furthermore, in reality, contact between materials at interfaces typically involves voids rather than ideal perfect contact, reducing the actual contact area and affecting heat conduction. To incorporate the effect of voids on contact area in interfacial thermal conductance predictions, we introduce a parameter S (interface contact coefficient) to correct the contact area. For perfect void-free interfaces, $S = 1$; for realistic interfaces with voids, $S < 1$. The actual interfacial thermal conductance G can be expressed as:

$$G = S \cdot G_m$$

where G_m is the interfacial thermal conductance calculated from the theoretical model, and S is the interface contact coefficient.

3. Results and Discussion

The phonon dispersion relations and DOS for metals (Al, Cu, Au) and semiconductors (Si, SiC) were calculated using the lattice dynamics software GULP [33], employing the Mei-Davenport potential [34] for Al, EAM potentials [35,36] for Cu and Au, the SW potential [37] for Si, and the Tersoff potential [38] for

SiC. The dispersion relations and DOS for GaAs and GaN were calculated using VASP combined with phonopy. The phonon dispersion relations and DOS for these three metals and four semiconductors are shown in Figures 1 [Figure 1: see original paper] and 2 [Figure 2: see original paper].

Figure 1. Phonon dispersion relations and density of states (DOS) of metals: (a) Al, (b) Cu, (c) Au.

Figure 2. Phonon dispersion relations and density of states (DOS) of semiconductors: (a) Si; (b) SiC; (c) GaAs; (d) GaN.

In Figures 1 and 2, the red curves represent the normalized DOS. Metals (Al, Cu, Au) have face-centered cubic structures with only one atom per primitive cell, so their dispersion relations contain only acoustic branches, with cutoff frequencies in descending order: Al (8.4 THz), Cu (8.1 THz), Au (3.8 THz). For semiconductor materials, the primitive cell contains more than one atom, so the dispersion relations include both acoustic and optical branches. Since the theoretical models consider only interactions between identical phonon modes j at the interface, we consider only acoustic branch contributions to interfacial thermal conductance for semiconductor materials. The acoustic branch cutoff frequencies in descending order are: SiC (20 THz), Si (13 THz), GaN (7.1 THz), GaAs (6.2 THz). The phonon group velocities v_j for each mode can be obtained from the phonon dispersion curves (detailed group velocities are provided in Supplementary Material I). Below, we demonstrate the calculation process for interfacial thermal conductance at Al/semiconductor (Si, SiC, GaAs, GaN) interfaces.

Using Equations (2) through (5), we calculate the phonon transmittance spectra for Al/semiconductor interfaces under three models: AMM, DMM, and MMM (with roughness values: 0.28 nm, 1.38 nm, 2.16 nm), as shown in Figure 3 [Figure 3: see original paper]. Similar calculations can be performed for Cu/semiconductor and Au/semiconductor interfaces (detailed spectra are provided in Supplementary Material II). For Al/Si, Al/GaAs, and Al/GaN interfaces, the phonon transmittance calculated by AMM is higher than that by DMM across most frequencies. This occurs because AMM assumes specular transmission at the interface without scattering, making transmittance probability dependent solely on acoustic impedance mismatch. Conversely, DMM assumes a completely disordered interface with fully diffuse scattering. For the Al/SiC interface, DMM yields higher transmittance than AMM due to the large acoustic impedance mismatch between the two materials, where DMM predictions exceed AMM results [29].

Figure 3 [Figure 3: see original paper]. Comparison of phonon transmittance spectra calculated by AMM, DMM and MMM (roughness: 0.28nm, 1.38nm, 2.16nm): (a) Al/Si interface; (b) Al/SiC interface; (c) Al/GaAs interface; (d) Al/GaN interface.

Substituting the phonon transport parameters and transmittance into Equation (1) yields the temperature-dependent interfacial thermal conductance curves.

Additionally, prior to theoretical modeling, we establish the relationship between interface contact coefficient S and interface roughness based on interfacial contact mechanics theory [39], as shown in Figure 4 [Figure 4: see original paper]. Here, $\eta_{\max}$ represents the cutoff radius of the interatomic empirical potential function for the materials on both sides of the interface. When interface roughness exceeds this value, the interface contact coefficient approaches zero; for the Al/Si interface, this value is 4.7 nm (values for other interfaces are provided in Supplementary Material III). The same methodology can be applied to obtain the S-roughness relationship for other metal/semiconductor interfaces.

Figure 4 [Figure 4: see original paper]. The relationship between interface contact coefficient S and roughness, where $\eta_{\max}$ is the cutoff radius of the interatomic empirical potential function of the materials on both sides of the interface. When the roughness of the interface is greater than this value, the interface contact coefficient is considered to approach 0, which is 4.7nm for Al/Si interface.

Substituting the coefficient S into Equation (7) allows calculation of theoretical model results at different temperatures and roughness values, as shown in Figure 5 [Figure 5: see original paper]. Comparison with experimental measurements for Al/Si interfaces demonstrates that MMM calculations agree well with experimental data.

Figure 5. Curves of interfacial thermal conductance predicted by AMM, DMM and MMM (roughness: 0.28nm, 1.38nm, 2.16nm) models as a function of temperature: (a) Al/Si interface, (b) Al/SiC interface, (c) Al/GaAs interface, (d) Al/GaN interface; The experimental values were obtained from measurements made by Hopkins [15] et al.

Figure 5 shows that interfacial thermal conductance gradually saturates with increasing temperature. During this process, phonon group velocity, DOS, and interface transmittance remain constant. The temperature dependence arises from the Bose-Einstein distribution. At low temperatures, only low-frequency phonons contribute to interfacial thermal conductance. As temperature increases, higher-frequency phonons are excited and participate in interfacial thermal transport, thereby increasing conductance. At sufficiently high temperatures, the number of excited phonons saturates, and further temperature increases do not activate additional phonons, causing the interfacial thermal conductance to reach saturation.

Similar procedures can be applied to calculate temperature-dependent interfacial thermal conductance curves for other metal (Cu, Au)/semiconductor (Si, SiC, GaAs, GaN) interfaces (detailed results are provided in Supplementary Material IV). Theoretical calculations employ the same method shown in Figure 4 to obtain contact coefficient S for different interfaces. The calculated interfacial thermal conductance values at various roughness levels are presented in Figure 6 [Figure 6: see original paper], demonstrating that for metal/semiconductor interfaces, interfacial thermal conductance decreases with increasing roughness,

consistent with previous studies [14,15,17,28].

Figure 6 [Figure 6: see original paper]. Interfacial thermal conductance of metal (Al, Cu, Au) and semiconductor (Si, SiC, GaAs, GaN) interfaces predicted by MMM model at 300 K, roughness values: 0.28nm, 1.38nm, 2.16nm.

The results show that Al/semiconductor and Cu/semiconductor interfaces exhibit similar predicted thermal conductance values, but differ significantly from Au/semiconductor interfaces. Al and Cu have nearly identical phonon dispersion relations and DOS, with similar phonon frequencies participating in interfacial thermal transport. However, Au has a lower phonon dispersion cutoff frequency, allowing only fewer low-frequency phonons to participate. Additionally, metal/semiconductor interfaces with Al and Cu generally exhibit higher thermal conductance because these metals have higher phonon dispersion cutoff frequencies that overlap more strongly with semiconductor DOS compared to Au. For metals with higher cutoff frequencies such as molybdenum (Mo) [40], chromium (Cr) [41], and nickel (Ni) [42], high interfacial thermal conductance can also be achieved; whereas metals with lower cutoff frequencies such as platinum (Pt) [42], ruthenium (Ru) [43], and tungsten (W) [44] yield relatively lower interfacial thermal conductance.

From the semiconductor perspective, interfaces with Si and GaN show higher thermal conductance for metal (Al, Cu)/semiconductor combinations, while SiC —which has high bulk thermal conductivity—exhibits lower interfacial thermal conductance. This occurs because SiC' s acoustic branch cutoff frequency is much higher than those of Al and Cu, whereas Si and GaN have acoustic branch cutoff frequencies closer to Al and Cu, resulting in greater DOS overlap and more phonons participating in interfacial transport. Semiconductors with lower acoustic branch cutoff frequencies such as zinc oxide (ZnO) [45], gallium oxide (Ga_2O_3) [46], and indium phosphide (InP) [47] yield lower interfacial thermal conductance. For GaAs, Au' s dispersion cutoff frequency is more similar, resulting in higher DOS overlap and thus greater Au/GaAs interfacial thermal conductance compared to other Au/semiconductor (Si, SiC, GaN) interfaces.

4. Summary and Outlook

In summary, this work proposes a simplified mixed mismatch model for predicting interfacial thermal conductance by considering the effects of interface roughness and structure. The validity of the simplified MMM is confirmed by comparing Al/Si interface predictions with experimental measurements. Based on this model, we calculate and predict interfacial thermal conductance between metals (aluminum, copper, gold) and semiconductors (silicon, silicon carbide, gallium arsenide, gallium nitride). The results show that metal/semiconductor interfacial thermal conductance increases with temperature but the rate of increase slows at higher temperatures. Furthermore, calculations incorporating interface structure effects demonstrate that interfacial thermal conductance decreases with increasing roughness. The simplified mixed mismatch model offers

the advantages of simplicity and accurate predictions, facilitating both interfacial thermal conductance prediction and comparison with experimental measurements.

References

[1] Wei N, Zhou C, Li Z, Ou B, Zhao K, Yu P, Li S, Zhao J 2022 Mater. Today Commun. 30 103147
[2] Monachon C, Weber L, Dames C 2016 Annu. Rev. Mater. Res., Vol 46 p433
[3] Cui Y, Li M, Hu Y 2020 J. Mater. Chem. C 8 10568
[4] Deng S, Xiao C, Yuan J, Ma D, Li J, Yang N, He H 2019 Appl. Phys. Lett. 115 101603
[5] Cahill D G, Braun P V, Chen G, Clarke D R, Fan S, Goodson K E, Keblinski P, King W P, Mahan G D, Majumdar A, Maris H J, Phillpot S R, Pop E, Shi L 2014 Appl. Phys. Rev. 1
[6] Scott E A, Gaskins J T, King S W, Hopkins P E 2018 APL Mater. 6
[7] Yang L, Wan X, Ma D, Jiang Y, Yang N 2021 Phys. Rev. B 103 155305
[8] Liu B, Khvesyuk V I, Barinov A A, Wang M 2022 Int. J. Mech. Sci. 218 106993
[9] Cahill D G, Braun P V, Chen G, Clarke D R, Fan S, Goodson K E, Keblinski P, King W P, Mahan G D, Majumdar A, Maris H J, Phillpot S R, Pop E, Shi L 2014 Applied Physics Reviews 1 011305
[10] Yang N, Luo T, Esfarjani K, Henry A, Tian Z, Shiomi J, Chalopin Y, Li B, Chen G 2015 J. Comput. Theor. Nanosci. 12 168
[11] Rustam S, Schram M, Lu Z, Chaka A M, Rosenthal W S, Pfaendtner J 2022 ACS Appl. Mater. Interfaces
[12] Zhang P, Yuan P, Jiang X, Zhai S, Zeng J, Xian Y, Qin H, Yang D 2018 Small 14
[13] Giri A, Hopkins P E 2019 Adv. Funct. Mater. 30
[14] Duda J C, Hopkins P E 2012 Appl. Phys. Lett. 100 111602
[15] Hopkins P E, Duda J C, Petz C W, Floro J A 2011 Phys. Rev. B 84
[16] Hopkins P E, Duda J C, Clark S P, Hains C P, Rotter T J, Phinney L M, Balakrishnan G 2011 Appl. Phys. Lett. 98
[17] Hopkins P E, Phinney L M, Serrano J R, Beechem T E 2010 Phys. Rev. B 82 085307
[18] Lee E, Zhang T, Yoo T, Guo Z, Luo T 2016 ACS Appl. Mater. Interfaces 8 35505
[19] Park W, Sood A, Park J, Asheghi M, Sinclair R, Goodson K E 2017 Nanoscale Microscale Thermophys. Eng. 21 134
[20] Liang Y, Zhang B, Liu Z, Liu W 2021 Int. J. Heat Mass Transfer 174
[21] Xu Y, Kato R, Goto M 2010 J. Appl. Phys. 108
[22] Nylander A, Hansson J, Nilsson T, Ye L, Fu Y, Liu J 2021 ACS Appl. Mater. Interfaces 13 30992
[23] Zhang Y, Ma D, Zang Y, Wang X, Yang N 2018 Front. Energy Res. 6
[24] Monachon C, Weber L, Dames C 2016 Annu. Rev. Mater. Res. 46 433
[25] Singh P, Seong M, Sinha S 2013 Appl. Phys. Lett. 102

[26] Hamaoui G, Horny N, Hua Z, Zhu T, Robillard J F, Fleming A, Ban H, Chirtoc M 2018 Sci Rep 8 11352
[27] Giri A, Gaskins J T, Donovan B F, Szwejkowski C, Warzoha R J, Rodriguez M A, Ihlefeld J, Hopkins P E 2015 J. Appl. Phys. 117
[28] Chen J, Xu X, Zhou J, Li B 2022 Rev. Mod. Phys. 94 025002
[29] Swartz E T, Pohl R O 1989 Rev. Mod. Phys. 61 605
[30] Kazan M, Bruyant A, Royer P, Masri P 2010 Surf. Sci. Rep. 65 111
[31] De Bellis L, Phelan P E, Prasher R S 2000 J. Thermophys. Heat Transfer 14 144
[32] Ziman J M 1960 Electrons and Phonons: The Theory of Transport Phenomena in Solids (Oxford University Press)
[33] Gale J D, Rohl A L 2003 Mol. Simul. 29 291
[34] Mei J, Davenport J W 1992 Phys. Rev. B 46 21
[35] Foiles S M, Baskes M I, Daw M S 1986 Phys. Rev. B 33 7983
[36] Johnson R A 1989 Phys. Rev. B 39 12554
[37] Stillinger F H, Weber T A 1985 Phys. Rev. B 31 5262
[38] Tersoff J 1988 Phys. Rev. B 38 9902
[39] Mulakaluri N, Persson B N J 2011 EPL 96
[40] Farber D L, Krisch M, Antonangeli D, Beraud A, Badro J, Occelli F, Orlikowski D 2006 Phys. Rev. Lett.
[41] Trampenau J, Petry W, Herzig C 1993 Phys. Rev. B 47 3132
[42] Dal Corso A 2013 J. Phys.: Condens. Matter 25 145401
[43] Koh Y R, Shi J, Wang B, Hu R, Ahmad H, Kerdsongpanya S, Milosevic E, Doolittle W A, Gall D, Tian Z, Graham S, Hopkins P E 2020 Phys. Rev. B 102
[44] Debernardi A, Alouani M, Dreyssé H 2001 Phys. Rev. B 63 064305
[45] Serrano J, Manjón F J, Romero A H, Ivanov A, Cardona M, Lauck R, Bosak A, Krisch M 2010 Phys. Rev. B 81
[46] Ghosh K, Singisetti U 2016 Appl. Phys. Lett. 109
[47] Fritsch J, Pavone P, Schroder U 1995 Phys. Rev. B 52 11326

Note: Figure translations are in progress. See original paper for figures.