First-principal Study and Experiment on Temperature-dependent Substitution Process of Si in $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ Solid Solution

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Abstract

High-pure $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ solid solutions were synthesized by using Ti, Si, Al and TiC powders in the range of 1473K to 1773 K. The microstructures and chemical compositions of all samples were characterized by X-rays diffraction (XRD) and scanning electron microscope (SEM). Microstructural analysis and mechanical properties test demonstrated that the $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ solid solutions exhibited highest relative density and mechanical properties when synthesized at 1773 K. In addition, it was worthy noted that experimentally determined lattice parameter c of $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ crystal decreased with the increasing of sintering temperature. The contents of Si and Al elements in solid solution were conducted by Vegard's Law. Gibbs energy differences (ΔG) of substitution process of Si (Si replace Al atoms) in $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ solid solutions at different temperatures were also listed. With the increase of temperature, the ΔG value was negative and decreased gradually, which means that the transformation from $\text{Ti}_3(\text{Si}_{\text{poor}}\text{Al}_{\text{rich}})\text{C}_2$ to $\text{Ti}_3(\text{Si}_{\text{rich}}\text{Al}_{\text{poor}})\text{C}_2$ was spontaneous and had a greater tendency in higher temperatures. By combined the experimental and calculational data, a possible mechanism of this transformation was determined.

Keywords: $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$, Solid solution; Sintering temperature; First-principle calculations; Substitution process.

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1. Introduction

MAX phase compounds (M is an early transition metal, A is an A group element, X is carbon or nitrogen) with the $P6_3/mmc$ space group, have attracted more attention in recent years due to the excellent combination of metallic and ceramic properties,^[1-5] including good thermal and electrical conductivity, low coefficient of thermal expansion and superior machinability. To date, more than 150 kinds of MAX phases have been discovered,^[6,7] most of which belong to 211, 312 and 413 phase. Ti_3SiC_2 is a part of the large family of ternary laminate compounds, with various synthesis methods such as pressureless,^[8] microwave sintering,^[9] hot pressing (HP)^[10-13] and spark plasma sintering (SPS).^[14-18] Sintering temperatures is a significant parameter in in-situ synthesis process, excessive temperature would cause decomposition of

Ti_3SiC_2 as well as generate TiC as an impurity. The sintering temperatures and contents (also mechanical properties if they are available) of Ti_3SiC_2 synthesized via different sintering methods are summarized in Table 1.

Solid solution modification method was often used to transform ternary MAX phase to quaternary, or even quinary compounds which at least contain two M, two A or two X elements, such as $(\text{Cr},\text{Ti})_3\text{AlC}_2$,^[19] $(\text{Zr},\text{Ti})_3\text{AlC}_2$,^[20] $\text{Ti}_2(\text{Al},\text{Sn})\text{C}$,^[21] $(\text{Ti},\text{Cu})_3(\text{Al},\text{Cu})\text{C}_2$,^[22] $(\text{Zr},\text{Ti})_2(\text{Al},\text{Sn})\text{C}$.^[23] Burr^[19] summarized the major advantages of quaternary MAX ceramics, indicating that they had new and outstanding mechanical properties compared with common MAX phases. As Si and Al elements have similar atomic radius, Al atoms often dissolved into Ti_3SiC_2 crystal inevitably, generating $\text{Ti}_3(\text{Si}_x\text{Al}_{1-x})\text{C}_2$ solid solution when Al was added as sintering additive via in-situ synthesis. Some research^[24-29] suggested that adding an appropriate amount of Al to initial powder mixtures can lower the sintering temperature, improve the yield and oxidation resistance of the products.

First-principles calculations are valuable to predict the properties and behaviors of crystalline materials.^[30,31] By analyzing electron-phonon coupling strengths obtained both in experiments and density functional calculations, it is

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Table 1. The synthesis methods and mechanical properties of Ti_3SiC_2 .

Method	Temperature/ K	Raw materials	Ti_3SiC_2 contents	Vickers' hardness (GPa)	Flexural strength (MPa)	Fracture toughness ($\text{MPa}\cdot\text{m}^{1/2}$)	Ref.
pressureless	1673	$\text{Ti}+2\text{TiC}+1.2\text{Si}+0.3\text{Al}$	91.30%	/	380	4.1	[8]
microwave	1753	$3\text{Ti}+1.15\text{Si}+2\text{C}$	98%	/	/	/	[9]
HP	1673	$3\text{Ti}+\text{Si}+2\text{C}+0.2\text{Al}$	93.70%	/	554.81	/	[10]
	1653	$4\text{Ti}+2\text{SiC}+\text{TiC}+0.2\text{Al}$	>99%	/	/	/	[11]
	1573	$3\text{Ti}+1.5\text{Si}+1.9\text{C}+0.5\text{Al}$	95.80%	/	/	/	[12]
	1873	$3\text{Ti}+1.2\text{Si}+2\text{C}$	>99%	4.32 ± 0.16	370	/	[13]
SPS	1523	$3\text{Ti}+\text{SiC}+\text{C}+0.15\text{Al}$	98.50%	6.32 ± 0.17	/	/	[14]
	1573	$\text{Ti}+2\text{TiC}+1.3\text{Si}$	85%	8.2	/	5.4	[15]
	1673	$\text{Ti}+2\text{TiC}+1.1\text{Si}+0.2\text{Al}$	>99%	7.31 ± 0.62	995	6.37 ± 0.77	[16]
		$2\text{Si}+3\text{TiC}$	87%	4.9		/	[17]
	1423	$\text{Ti}+2\text{TiC}+1.1\text{Si}+0.2\text{Al}$	98.90%	8.47 ± 0.31	/	/	[18]
		$\text{Ti}+2\text{TiC}+1.2\text{Si}+0.2\text{Al}$	>99%	6.94 ± 0.51	/	/	

predicted that Ta_2AlC might be a new superconductive MAX phase.^[32] Lane^[33] investigated the thermal expansions and temperature-dependent crystal structures of Ti-Al-C phase diagram in the temperature range of 373–1373K and demonstrated that thermal expansions of Ti_2AlC , Ti_3AlC_2 and $\text{Ti}_5\text{Al}_2\text{C}_3$ were higher in the *c* direction in contrast with *a* direction. Lu^[34] reported the substitution behavior of Si atoms in the Ti_2AlC ceramics and calculated the formation energy of this process to be -0.37 eV.

In this study, high-purity $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ solid solutions were synthesized at 1473, 1573, 1673 and 1773K. As the increase of sintering temperature, the density and mechanical properties of $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ were improved significantly. At the same time, the content of Al decreased rapidly in $\text{Ti}_3(\text{Si},\text{Al})\text{C}_2$ crystal. This phenomenon was caused by the fracture of Ti-Al bonds, which were more susceptible to high temperatures compared with Ti-Si bonds, leading to this transformation process from $\text{Ti}_3(\text{Si}_{\text{poor}}\text{Al}_{\text{rich}})\text{C}_2$ to $\text{Ti}_3(\text{Si}_{\text{rich}}\text{Al}_{\text{poor}})\text{C}_2$ solid solutions.

2. Materials and methods

2.1 Experimental method

The $\text{Ti}_3(\text{Si}_x\text{Al}_{1-x})\text{C}_2$ bulk were prepared via hot-pressing sintering using molar ratio 1.0Ti/1.2Si/0.3Al/2.0TiC powders at 1473, 1573, 1673 and 1773K respectively. The pressure was maintained at 30 MPa for 1.5 h at the specified temperatures. Finally, the sintered samples were allowed to cool naturally to room temperature before removing from the furnace. The obtained samples were polished by using SiC powder and then cleaned via ultrasonication. The phase compositions of the obtained samples were determined by XRD (D8 ADVANCE, Bruker). Microstructural investigations were performed by SEM (JSM-7610F, JEOL, Japan) with an energy dispersive spectroscopy (EDS) after coating Au on measurement surface for 30S. The density of samples were determined by using the

Archimedes water immersion method. The flexural strength and fracture toughness of the samples were measured using the three-point bending method on an electromechanical universal testing machine (CMT5504, MTSSYSTEMS, China) with a cross-head speed of 0.5 mm/min and a span of 30 mm. The hardness of the samples was determined using a Vickers hardness tester (HV-100IS, China) at a load of 10 N for 20 S.

2.2 Theoretical method

First-principles calculations were performed by using the plane-wave CASTEP codes based on the density functional theory (DFT) approach. The electron exchange-correlation was described using the GGA-PBE function. The plane-wave ultrasoft pseudopotential methods were exploited to present the interactions between the electrons and the ion cores and the cut-off energy was 450 eV. The virtual crystal approximation (VCA) and supercell (SC) methods were employed to construct the solid solution crystal model. VCA was introduced by assigning partial occupancies to each atomic site and SC was performed by enlarging $2\times 2\times 1$ supercell (48 atoms). K-points were determined to be $8\times 8\times 2$ for VCA and $4\times 4\times 2$ for SC. All models were relaxed until the forces on each atom were <0.03 eV/Å, and the stress on each atom was converged to 0.05 GPa. The maximum atom displacement was set at 0.001 Å, and the total energy changes during the optimization finally converged to 10^{-5} eV/atom. Phonon dispersion calculations were performed by using the finite displacement method and the supercell was defined using a cutoff radius of 5.0 Å. Gibbs energy was evaluated by employing the quasiharmonic approximation (QHA). The modelling for first-principle calculations were shown in Supplementary materials.

3. Results and discussion

3.1 Composition and microstructural analysis

Fig. 1 XRD data for samples 1-4 with 2 theta (a) 25-80 degree; (b) 38-43 degree.

Samples 1-4 were fabricated at 1473, 1573, 1673 and 1773 K respectively. The phase compositions of the obtained ceramics were analyzed through XRD (Fig. 1a), where strong peaks corresponding to $\text{Ti}_3(\text{Si,Al})\text{C}_2$ were clearly shown and different crystal planes were also indexed. No obvious peaks of Ti-Si/Al alloy and TiC were discovered, indicating the complete reaction between 1473 and 1773 K.

SEM images (see Fig. 2) revealed a significant change of the microstructures as increasing the sintering temperature. Large holes and relatively small grains were presented in Fig. 2a. As the sintering temperature up to 1573 K, the number of holes and small grains reduced obviously (Fig. 2b). Samples 3

and 4 (Fig. 2c and 2d) exhibited grown grains with no obvious micropores, as well as grain boundaries were clearer than samples 1 and 2.

3.2 Mechanical properties

Fig. 3a showed the relative density of samples 1-4. The density of samples improved rapidly with the sintering temperatures increasing, which were determined to 92.7%, 95.5%, 98.9% and 99.2% at the temperatures of 1473 K, 1573 K, 1673 K and 1773 K, respectively. This result was in accordance with the microstructural analysis, that was, appropriate high temperatures (1673-1773 K). would

Fig. 2 SEM images of (a) sample 1; (b) sample 2; (c) sample 3; (d) sample 4.

Fig. 3 (a) relative density and Vickers' hardness; (b) flexural strength and fracture toughness of samples 1-4.

accelerate the growth of crystals, decrease porosity and improve densification, which was beneficial for promotion of density.

The mechanical properties including Vickers' hardness, flexural strength, and fracture toughness of samples 1-4 were described in Fig. 3a and 3b. The value of mechanical properties improved as the increasing of sintering temperature, the optimized of which were determined to 5.76 GPa, 433 MPa and 6.74 MPa.m^{1/2} at 1773 K for Vickers' hardness, flexural strength, and fracture toughness respectively. It was clearly that high densification could enhance the mechanical properties significantly. The hardness value for Ti₃SiC₂ reported by Ghosh *et. al*^[14] was 6.32 GPa, while it contained 98.5% Ti₃SiC₂ and 1.5% TiC, which would increase the hardness as a hard impurity phase. Islak^[16] *et. al* fabricated purity Ti₃SiC₂ bulk by SPS at 1673K, with Vickers' hardness of 7.31±0.62 GPa and fracture toughness of 6.37±0.77 MPa.m^{1/2}.

3.3 Calculation for Ti₃(Si,Al)C₂ solid solution

Partial enlarged drawing of (104), (008) and (105) planes were shown in Fig. 1b. All the peaks shifted right to a bigger 2 theta degree with the increasing of temperature, which meant that the lattice parameter of Ti₃(Si,Al)C₂ declined. Because the radii of the Si atoms were smaller than Al, the cause for this phenomenon is the substitution behavior of Si to replace Al site in Ti₃(Si,Al)C₂ solid solution.

To investigate the influence of sintering temperature on the solid solution, the lattice parameters of Ti₃(Si,Al)C₂ and contents of Si/Al elements were calculated by using the spectrum fitting method and first-principle calculations. Vegard's law is an empirical rule, stating that the lattice parameters can be calculated from a linear interpolation of its constituent elements fraction. Herein, supercell (SC) and virtual crystal approximation (VCA) methods were used to reveal the relationship between lattice parameters and Si/Al contents. Because of the similar *a* value in Ti₃SiC₂ and Ti₃AlC₂ crystal, it is unsuitable for calculating Si/Al contents, *c* value

was adopted to further calculate. The lattice parameter *c* was obtained by optimizing the geometry of Ti₃(Si_xAl_{1-x})C₂ modeling. (*x*=0, 0.125, 0.25, 0.5, 0.75, 0.875, 1). Combined SC and VCA methods, Fig. 4 plotted the lattice parameter *c* as a function of the atomic ratio of Al in Ti₃(Si,Al)C₂ solid solution. A good linear relationship was shown for VCA methods. However, when *x*=0.125, 0.25 and 0.5 for SC method, it caused a markedly higher deviation. By summarizing the analysis above, VCA was adopted to fit linear to calculate the contents of Si and Al, which can be shown in Eq.(1),

$$y = 1.1263x + 17.615 \quad (1)$$

where *y* represents lattice parameter *c* and *x* is the molar ratio of Al, and the results are listed in Table 2.

Fig. 4 The calculated lattice parameters with various Al content of Ti₃(Si_xAl_{1-x})C₂ modeling by SC and VCA methods.

Table 2 The calculated fraction of Al in solid solution at different temperatures.

Temperature/K	1473	1573	1673	1773
<i>c</i> /Å	17.8256	17.8087	17.7321	17.6837
Al/ at%	18.7	17.2	10.4	6.1

It was found that at 1473 K, the fraction of Al in $Ti_3(Si,Al)C_2$ was very close to that in raw materials (20 at %), indicating that almost all of Al element would present in $Ti_3(Si,Al)C_2$ crystal. As the temperature increased, masses of Al atoms will be substituted by Si, causing that Al content reduced rapidly and only 6.1 at% existed in $Ti_3(Si,Al)C_2$ at 1773K. The substitution process of Si atoms can be conducted by the following reactions:

The formation energy can be evaluated according to the following Eq:

$$E_f = E_{Ti_3(Si_{x+y}Al_{1-x-y})C_2} + yE_{Al} - E_{Ti_3(Si_xAl_{1-x})C_2} - yE_{Si} \quad (3)$$

To make the calculated process close to the real experiments, we simulated the transformation changed from $Ti_3(Si_{0.75}Al_{0.25})C_2$ to Ti_3SiC_2 . The modeling of $Ti_3(Si_{0.75}Al_{0.25})C_2$ was constructed by $Ti_3(Si,Al)C_2$ unit-cell enlarged by $2 \times 2 \times 1$, containing 24 Ti, 6 Si, 2Al and 16 C

Fig. 5 Formation energy for substitution of Si.

atoms in total. This process was displayed in Fig. 5. The formation energy (Fig. 5) would up to 1.78 eV once the Al vacancy emerged in $Ti_3(Si_{0.75}Al_{0.25})C_2$ modeling.

Fig. 6 SEM and EDS images of grain boundary.

Subsequently, it decreased to -0.38eV when Si atom occupied the vacancy to form $Ti_3(Si_{0.875}Al_{0.125})C_2$ structure. The negative formation energy indicated that substitution of Si was spontaneous and could improve the structural stability of the solid solution. Similar to the previous step, the most stable structure Ti_3SiC_2 formed after another Si atom replaced Al atom, and the formation energy value was -0.42 eV. Because the sintering was processed over 1473K, the phonon calculations were used to reveal the Gibbs energy difference of the above transformation:

The results were listed in Table 3.

Table 3 Gibbs energy difference of reaction (4) at different temperatures.

Temperature (K)	1473	1573	1673	1773
ΔG (KJ/mol)	-13.16	-13.57	-14.23	-15.85

With the temperature increased, the ΔG of reaction (4) decreased from -13.16 to -15.85 KJ/mol, suggesting that Si atoms were more preferred to replace Al atoms at higher temperatures. Ti-Al and Ti-Si bonds properties were evaluated by calculating single point energy for Ti, Si, Al, Ti-Al, and Ti-Si model, which were shown in Table 4.

Table 4 Bond length and energy for Ti-Si and Ti-Al bond in $Ti_3(Si,Al)C_2$ solid solution.

	Bond length (Å)	Bond energy (eV)
Ti-Si	2.6784	3.7146
Ti-Al	2.9011	2.1226

Ti-Al bond has a larger length and lower energy than Ti-Si bond, as the temperature increased, Ti-Al bond is particularly susceptible to break, forming Al vacancy in solid solution. Afterward, Si atoms fill the vacancy to generate a stronger Ti-Si bond. It was worthwhile pointing out that aggregation of Al elements was found in grain boundary (see Fig. 6), which was mainly attributed to the segregation.

Table 5. The calculated elastic constants (GPa), bulk modulus B(GPa), shear modulus G (GPa), Yong's modulus E (GPa) and Poisson's ratio σ .

		C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E	σ
Ti ₃ SiC ₂	this work	365.3	87.8	101.3	353.4	158.2	184.8	143.6	342.3	0.19
	Ref.[35]	364.2	95.4	112.5	351.8	157.2	191.2	139.6	336.9	0.2
	Ref.[36]	370	99.2	110.6	349.4	150.6	192.2	138.1	334.3	0.2
Ti ₃ AlC ₂	this work	355.1	73.4	68.8	296.5	126.7	158.2	131.8	309.5	0.19
	Ref.[35]	355.2	82.2	76.6	292.4	119.3	163	125.8	300.2	0.2
	Ref.[36]	358.1	83.9	74.8	292.6	122	163.1	127.3	303.1	0.2
Ti ₃ (Si _{0.875} Al _{0.125})C ₂	this work	364.3	83.2	94.5	338.2	152.6	178.4	141.2	336.6	0.19
Ti ₃ (Si _{0.75} Al _{0.25})C ₂	this work	362.7	80.5	88.1	323.6	145.9	173.6	137.5	326.3	0.19

Elastic constants, bulk modulus, shear modulus, Yong's modulus and Poisson's ratio of Ti₃SiC₂, Ti₃AlC₂, Ti₃(Si_{0.875}Al_{0.125})C₂ and Ti₃(Si_{0.75}Al_{0.25})C₂ were calculated. As shown in Table 5, for pure Ti₃SiC₂ and Ti₃AlC₂, the calculated values in this work were in good agreement of other theoretical results.^[35,36] By analyzing the calculated data, it could be deduced that the elastic properties of solid solutions would enhance obviously as the increasing of Si percentage at A sites. Thus, a proper higher temperature would play a positive role in improving mechanical properties due to formation of Ti₃(Si_{rich}Al_{poor})C₂ solid solutions.

Fig. 7 The mechanism of substitution process of Si atoms in Ti₃(Si,Al)C₂ crystal.

4. Conclusion

In summary, high-pure Ti₃(Si,Al)C₂ solid solutions were fabricated at different sintering temperatures via in-situ synthesis. The influence of sintering temperature was discussed both by experiments and calculations. The following conclusions were drawn:

(1) High-purity Ti₃(Si,Al)C₂ solid solutions without impurity of TiC were synthesized by hot-pressing in the range of 1473K to 1773K using 1.0Ti/1.2Si/0.3Al/2.0TiC powders as raw materials.

(2) Sintering temperature significantly influenced the contents of Si and Al in Ti₃(Si,Al)C₂. That was, the percentage of Si would increase gradually at higher temperature. The mechanism of this phenomenon was attributed to the substitution behavior of Si atoms in Ti₃(Si,Al)C₂ solid solution (Fig. 7). Due to the lower bond energy, Ti-Al bond would prefer to fracture in high temperature, causing dissociative Al atoms and vacancy in the previous site. Subsequently, unreacted Si atoms would occupy the site to form Ti-Si bonds, and the extra Al atoms were likely to segregate in grain boundaries.

(3) Microstructural analysis, mechanical properties test and elastic constants data demonstrated that suitable higher sintering temperatures were beneficial to mechanical properties of Ti₃(Si,Al)C₂ solid solution. Experimentally, high-temperature promoted crystal growth, removed holes and increased densification. Moreover, from theoretical perspective, it improved the elastic constants and modulus by formation of Ti₃(Si_{rich}Al_{poor})C₂ solid solutions.

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Conflict of Interest

There is no conflict of interest.

Supporting Information

Not applicable

References

- [1] C. Lu, L. Sun, J. Zhang, Q. Qi, G. Hug, *Ceram. Int.*, 2017, **43**, 8579-8584, doi: 10.1016/j.ceramint.2017.03.113.
- [2] O. Dezellus, B. Gardiola, J. Andrieux, S. Lay, *Scripta Mater.*, 2015, **104**, 17-20, doi: 10.1016/j.scriptamat.2015.03.015.
- [3] W. Yu, J. Guénolé, J. Ghanbaja, M. Vallet, A. Guitton, *Scripta Mater.*, 2021, **191**, 34-39. doi: 10.1016/j.scriptamat.2020.09.007.

- [4] M. A. Hadi, S. R. G. Christopoulos, A. Chroneos, S. H. Naqib, A.K.M.A. Islam, *Mater Today Commun.*, 2020, **25**, doi: 10.1016/j.mtcomm.2020.101499.
- [5] P. Yao, Y. Qian, W. Li, C. Li, J. Zuo, J. Xu, M. Li, *Ceram. Int.*, 2020, **46**, 22919-22926, doi: 10.1016/j.ceramint.2020.06.065.
- [6] C. Magnus, D. Cooper, J. Sharp, W.M. Rainforth, *Wear*, 2019, **438**, doi: 10.1016/j.wear.2019.203013.
- [7] B. Velasco, E. Gordo, L. Hu, M. Radovic, S.A. Tsipas, *J. Alloy. Compd.*, 2018, **764**, 24-35, doi: 10.1016/j.jallcom.2018.06.027.
- [8] K. Sato, M. Mishra, H. Hirano, C. Hu, Y. Sakka, *J. Am. Ceram. Soc.*, 2014, **97**, 1407-1412, doi: 10.1111/jace.12903.
- [9] Q. Wang, C. Hu, S. Cai, Y. Sakka, S. Grasso, Q. Huang, *Int. J. Appl. Ceram. Technol.*, 2014, **11**, 911-918, doi: 10.1111/ijac.12065.
- [10] J. Wang, A. Li, S. Wang, H. Zeng, *Ceram. Int.*, 2012, **38**, 5967-5971, doi: 10.1016/j.ceramint.2012.04.049.
- [11] M. C. Peng, X. L. Shi, Z.W. Zhu, M. Wang, Q.X. Zhang, *Ceram. Int.*, 2012, **38**, 2027-2033, doi: 10.1016/j.ceramint.2011.10.038.
- [12] X. H. Li, L. Xu, Q.Y. Chen, X.X. Cao, L. X. Liu, Y. Wang, H. B. Zhang, C. Meng, Q. Wu, *High Pressure Res.*, 2018, **38**, 440-447, doi: 10.1080/08957959.2018.1501045.
- [13] Y. Luo, W. Pan, S. Li, J. Chen, R. Wang, J. Li, *Mater. Lett.*, 2002, **52**, 245-247, doi: 10.1016/S0167-577X(01)00401-3.
- [14] N. C. Ghosh, S. P. Harimkar, *Ceram. Int.*, 2013, **39**, 6777-6786, doi: 10.1016/j.ceramint.2013.02.008.
- [15] M.A. El Saeed, F.A. Deorsola, R.M. Rashad, *Int. J. Refract. Met. H.*, 2013, **41**, 48-53, doi: 10.1016/j.ijrmhm.2013.01.016.
- [16] B. Y. Islaka, E. Ayasb, *Ceram. Int.*, 2019, **45**, 12297-12306, doi: 10.1016/j.ceramint.2019.03.144.
- [17] F. Turki, H. Abderrazak, F. Schoenstein, M. Abdellaoui, N. Jouini, *J. Alloy. Compd.*, 2017, **708**, 123-133, doi: 10.1016/j.jallcom.2017.02.304.
- [18] A. Pourebrahim, H. Baharvandi, H. Foratirad, N. Ehsani, *J. Alloy. Compd.*, 2019, **789**, 313-322, doi: 10.1016/j.jallcom.2019.03.062.
- [19] P. A. Burr, D. Horlait, W. E. Lee, *Mater. Res. Lett.*, 2017, **5**, 144-157, doi: 10.1080/21663831.2016.1222598.
- [20] E. Z. Solvas, M. A. Hadi, D. Horlait, D. C. Parfitt, A. Thibaud, A. Chroneos, W.E. Lee, *J. Am. Ceram. Soc.*, 2017, **100**, 3393-3401, doi: 10.1111/jace.14870.
- [21] C. L. Yeh, C.H. Chiang, *Ceram. Int.*, 2015, **41**, 6263-6268, doi: 10.1016/j.ceramint.2015.01.048.
- [22] M. Nechiche, V. Gauthier-Brunet, V. Mauchamp, A. Joulain, T. Cabioc'h, X. Milhet, P. Chartier, S. Dubois, *J. Eur. Ceram. Soc.*, 2017, **37**, 459-466, doi: 10.1016/j.jeurceramsoc.2016.09.028.
- [23] B. Tunca, T. Lapauw, R. Delville, D.R. Neuville, L. Henne, D. Thiaudiere, T.Ouisse, J. Hadermann, J. Vleugels, K. Lambrinou, *Inorg. Chem.*, 2019, **58**, 6669-6683, doi: 10.1021/acs.inorgchem.9b00065.
- [24] X. Xu, T.L. Ngai, Y. Li, *Ceram. Int.*, 2015, **41**, 9626-9631, doi: 10.1016/j.ceramint.2015.02.088.
- [25] H.B. Zhang, Y.C. Zhou, Y.W. Bao, M.S. Li, J.Y. Wang, *J. Eur. Ceram. Soc.*, 2006, **26**, 2373-2380, doi: 10.1016/j.jeurceramsoc.2005.04.010.
- [26] J. Q. Zhu, B. C. Mei, X. W. Xu, J. Liu, *Mater. Lett.*, 2004, **58**, 588-592, doi: 10.1016/S0167-577X(03)00567-6.
- [27] A. Pourebrahim, H. Baharvandi, H. Foratirad, N. Ehsani, *J. Alloy. Compd.*, 2018, **730**, 408-416, doi: 10.1016/j.jallcom.2017.10.018.
- [28] H. B. Zhang, Y. C. Zhou, Y. W. Bao, M. S. Li, *Acta Mater.*, 2004, **52**, 3631-3637, doi: 10.1016/j.actamat.2004.04.015.
- [29] H. B. Zhang, X. Wang, C. Berthold, K.G. Nickel, Y.C. Zhou, *J. Eur. Ceram. Soc.*, 2009, **29**, 2097-2103, doi: 10.1016/j.jeurceramsoc.2008.12.010.
- [30] A. Togo, I. Tanaka, *Scripta Mater.*, 2015, **108**, 1-5, doi: 10.1016/j.scriptamat.2015.07.021.
- [31] M. Stumpf, J. Biggemann, T. Fey, K. Kakimoto, P. Greil, *Ceram. Int.*, 2018, **44**, 15747-15753, doi: 10.1016/j.ceramint.2018.05.249.
- [32] H. M. Xiang, J. M. Wang, Y. Chen, J. Y. Wang, Y. C. Zhou, *J. Raman Spectrosc.*, 2014, **45**, 202-207, doi: 10.1002/jrs.4441.
- [33] N. J. Lane, S.C. Vogel, E.N. Caspi, M.W. Barsoum, *J. Appl. Phys.*, 2013, **113**, 183519, doi: 10.1063/1.4803700.
- [34] C. Lu, K. Piven, Q. Qi, J. Zhang, G. Hug, A. Jankowiak, *Acta Mater.*, 2018, **144**, 543-551, doi: 10.1016/j.actamat.2017.11.002.
- [35] J. Nie, S. Liu, X. Zhan, L. Ao, L. Li, *Physica B.*, 2019, **571**, 105-111, doi: 10.1016/j.physb.2019.06.052.
- [36] W. Y. Ching, Y. X. Mo, S. Aryal, P. Rulis, *J. Am. Ceram. Soc.*, 2013, **96**, 2292-2297, doi: 10.1111/jace.12376.

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