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Molten Salt Synthesis of Nanolaminated Sc_2SnC MAX Phase

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Abstract: The MAX phases are a family of ternary layered material with both metal and ceramic properties, and it is also precursor materials for synthesis of two-dimensional MXenes. The theory predicts that there are more than 600 kinds of stable ternary layered MAX phase materials. Now, more than 80 kinds of ternary layered MAX phases that the M-site elements are mainly from early transition metal have been experimental synthesized, but few researches are reported on MAX phases where M is a rare earth element. In this study, Sc, Sn and C powders were used as raw materials to synthesize a novel ternary Sc_2SnC MAX phase *via* molten salt method. Phase composition and microstructure of Sc_2SnC were confirmed by X-ray diffraction, scanning electron microscope and X-ray energy spectrum analysis. And, structural stability, lattice parameters, mechanical and electronic properties of Sc_2SnC were investigated *via* density functional theory. The theoretical results show that Sc_2SnC is thermodynamically stable, and the Sc_2SnC is metallic in nature where the contribution from Sc-3d states dominates the electronic conductivity at the Fermi level. This study provides a route to explore more unknown ternary layered rare earth compounds $Re_{n+1}SnC_n$ (Re=Sc, Y, La-Nd, n=1) and corresponding rare earth MXenes.

Key words: MAX phases; nanolaminated; scandium; density-functional theory calculation

The MAX phases are a family of nanolayered ternary carbides or nitrides with a hexagonal lattice structure ($P6_3/mmc$), the chemical formula is $M_{n+1}AX_n$ (where M is an early transition metal; A is an element mainly from 13–16; and X is carbon or/and nitrogen, n=1–3)[1-3]. Generally, the heterodesmic feature of MAX phases contributes to a unique combination of both metallic and ceramic properties, which have been investigated as promising candidates for structural applications in many fields[4-7]. Moreover, MAX phases are used as a precursor to synthesize two-dimensional (2D) MXene with many attractive physical and chemical properties, and show promise in a broad range of applications, notably electrochemical energy storage[8-11]. Due to the continuing efforts from the scientific community, about 155 MAX phases have been reported so far, including some novel MAX phases that A-site elements are late transition metals[12-16]. The theoretical studies have predicted around 665 ternary MAX phases that could be experimentally synthesized[17], for example, the ones which M site element is rare earth Sc.

As previous reported, Sc_2InC was listed as one of possible stable MAX phases[1,3], where the structure, properties and potential applications are investigated *via* theoretical predictions[18-20], but not been experimentally identified yet. The Sc_2InC is expected to be a promising candidate for optoelectronic devices for the visible light and ultraviolet regions, as well as coating materials to avoid solar heating[20]. In addition, theoretical calculations indicate that the Sc_2CT_2 (T= F, OH) MXenes can be promising candidate materials for the next generation electronic devices[21]. Kuchida, *et al*[22] focused on non-transition metal M_2AX compounds which embody Sc, Y, and Lu atoms in M site, however, only polycrystalline sample of Lu_2SnC was reported. As a result, the study of new MAX phases taking Sc as M site element is an

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intriguing and challenging work.

Now, the common methods to synthesize MAX phases are hot pressing (HP) and spark plasma sintering (SPS). Compared to HP and SPS, the molten salt method is a simple and cost-effective route for preparing MAX phase powders. As a high-temperature ionic solvent, the molten salt bath offers high solvation power and liquid environment for reactants that will greatly facilitate the mass transport and nucleation processes, thus need lower synthesis temperature and bold time[23]. Some MAX phases (*e.g.* Ti_3SiC_2, Ti_3AlC_2, V_2AlC, Cr_2AlC) have been synthesized by molten salt method[24-28]. In the present work, we synthesized a MAX phase of Sc_2SnC in molten salts environment where the Sc element belongs to rare earth. The crystal structure and chemical composition were confirmed by XRD and SEM-EDS, respectively. Furthermore, the structure stability, electronic structure and mechanical properties of Sc_2SnC are also be investigated *via* density functional theory (DFT).

1 Experimental

The raw materials used to prepare the MAX phase are scandium (Hunan Rare Earth Metal Materials Research Institute, Hunan, China; ~48 μm (300 mesh), 99.5wt% purity), tin (Target Research Center of General Research Institute for Nonferrous Metals, Beijing, China, ~48 μm (300 mesh), 99.5wt% purity), graphite (Qingdao Tianshengda Graphite Co. Ltd, Shandong, China; ~48 μm (300 mesh), 99wt% purity), sodium chloride (Aladdin Industrial Co. Ltd, Shanghai, China; NaCl, 99.5wt% purity), potassium chloride (Aladdin Industrial Co. Ltd, Shanghai, China; KCl, 99.5wt% purity).

The powders were mixed in a stoichiometric ratio of Sc : Sn : C=2 : 1.1 : 1 (Due to the melting point of Sn is relatively low, we increased the content ratio of tin for compensating the weight loss of tin at a high temperature, as in the preparation of $V_2(Sn,A)C$ MAX phases)[16]. The starting powders of Sc, Sn and graphite are mixed with inorganic salt (NaCl + KCl), and the mole ratio of (Sc + Sn + C) : (NaCl + KCl) was 1 : 10, and the mole ratio of (NaCl : KCl) was 1 : 1. After ground for 10 min, the powder mixture was put into an aluminum oxide boat, and then moved to a tube furnace and heated to 1000 ℃ for 3 h at heating rate of 5 ℃/min under argon atmosphere, respectively. After the reaction was finished, the product was washed, filtered and dried at 40 ℃ in vacuum; and the excess Sn element was removed by ferric chloride (Aladdim Industrial Co. Ltd, Shanghai, China; $FeCl_3$, 99.5wt% purity).

The phase composition of the samples was determined by X-ray diffraction (XRD, D8 Advance, Bruker AXS, Germany) with Cu K_α radiation. X-ray diffraction patterns were collected at a step size of 0.02° (2θ) with a collection time of 1 s per step. The microstructure and chemical composition were observed by scanning electron microscope (SEM, QUANTA 250 FEG, FEI, USA) equipped with an energy-dispersive spectrometer (EDS), and the EDS values were fitted by XPP (extended Puchou/Pichoir).

Density functional theory (DFT) calculations were programmed in the CASTEP code[29-30], using the generalized gradient approximation (GGA) as implemented in the Perdew-Breke-Ernzerhof (PBE) functional[31-32]. Phonon calculations were carried out to evaluate the dynamical stability using the finite displacement approach, as implemented in CASTEP[33-34]. The equation $E=(E_{broken}-E_{bulk})/S$[13] was adopted to calculate the cleavage energy E, where E_{bulk} and E_{broken} represent the total energies of bulk MAX and the cleaving structures respectively with a 1 nm vacuum separation in the corresponding M and A atomic layers, and S is the cross- sectional surface area of the MAX phase materials. The Rietveld refinement of powder XRD pattern of Sc_2SnC was by Total Pattern Solution (TOPAS-Academic V6) software.

2 Results and discussion

2.1 Phase analysis of the Sc_2SnC

Fig. 1(a) shows the XRD pattern of as-prepared powders synthesized at 1000 ℃ for 3 h, has characteristic peaks at 2θ~12°, 24°, 36°, which neither belong to Sn nor other compounds, indicating that a new MAX phase of Sc_2SnC is synthesized (also with minor amount of Sn metal as by-product). In comparison with experimental result, the simulated XRD pattern of Sc_2SnC in Fig. 1(b), the peaks positioned at 2θ =12.174°, 24.517°, 36.277°, *etc.*, consist with the experimental peak positions in Fig. 1(a), which further validates the formation of the new MAX phase Sc_2SnC.

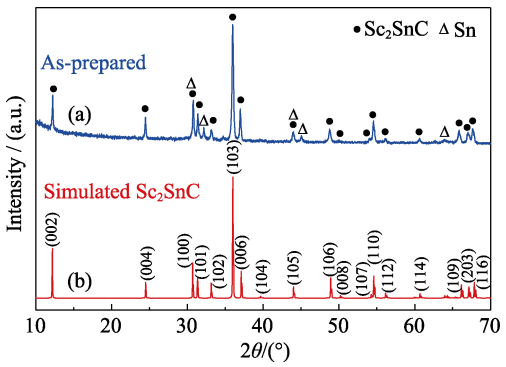

Fig. 1 Comparison of XRD patterns between (a) powders synthesized through the reaction between Sc, Sn, and C mixtures, and (b) the simulated one of Sc_2SnC

XRD pattern is important for phase identification and structure analysis. Because no XRD pattern of Sc_2SnC was available in previous literatures, the Rietveld refinement of powder XRD pattern of Sc_2SnC was conducted. As shown in Fig. 2, the blue crosses represent the experimental diffraction profile (the Sn metal was remove by $FeCl_3$ solution), while the red solid line denotes the theoretical pattern. The theoretical Bragg diffraction positions of Sc_2SnC are marked as red line. The gray curve is the deviation between calculated and experimental XRD patterns. The obtained reliability factors are R_p=8.56% and R_{wp}=11.19%, respectively, indicating good agreement between model and measured data. The space group of Sc_2SnC is $P6_3/mmc$ (194), and the lattice constants measured from XRD pattern are a=0.33692 nm and c=1.46374 nm, respectively. The difference between theoretical calculation and the Rietveld refinement is probably ascribed to the existence of defects in the crystal structure, as the case of V_2SnC in the previous report[35]. The atomic positions of Sc_2SnC determined from the Rietveld refinement are listed in Table 1.

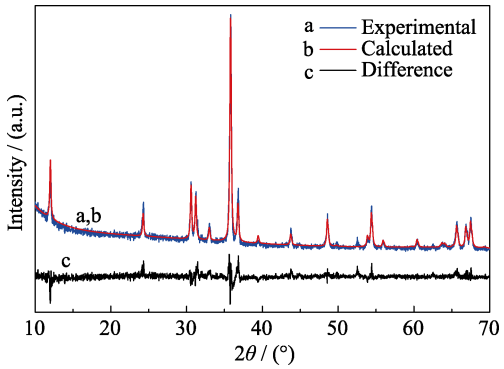

Fig. 2　Comparison between experimental (blue line) and calculated XRD (red line) pattern of Sc_2SnC

Table 1　Atomic positions in Sc_2SnC determined from the Rietveld refinement

Site	Element	x	y	z	Symmetry	Wyckoff symbol
M	Sc	1/3	2/3	0.5786	3m	4f
A	Sn	1/3	2/3	0.2500	$\bar{6}$m2	2d
X	C	0	0	0	$\bar{3}$m	2a

2.2　Microstructural of the Sc_2SnC

It is well known that MAX phases crystallize in hexagonal structures and their grains are generally layered hexagonsin morphology[1]. To confirm that Sc_2SnC has a similar microstructure, the microstructure of as-prepared powder was observed by SEM. It can be seen from Fig. 3(a) that Sc_2SnC exhibits the microstructure of typical thin hexagons. EDS equipped in SEM detected all constitutive elements (Sc, Sn and C) within these particles (as shown in Fig. 3(b)). Although the EDS analysis is semi-quantitative and the accurate determination of light elements like C is difficult, the relative atomic ratio of (Sc : Sn : C) could be revealed by EDS as about (2 : 1 : 1), consistent with the stoichiometry of 211 MAX phases. The elemental mapping of Sc, Sn and C corroborated that all of these three elements have the same distribution. The above results further confirm that the new MAX phase compound Sc_2SnC is experimentally synthesized.

2.3　DFT results

The structural analysis of Sc_2SnC phase was carried out *via* DFT calculations. Fig. 4(a) shows the ternary-layered carbide crystal structure of Sc_2SnC; and the

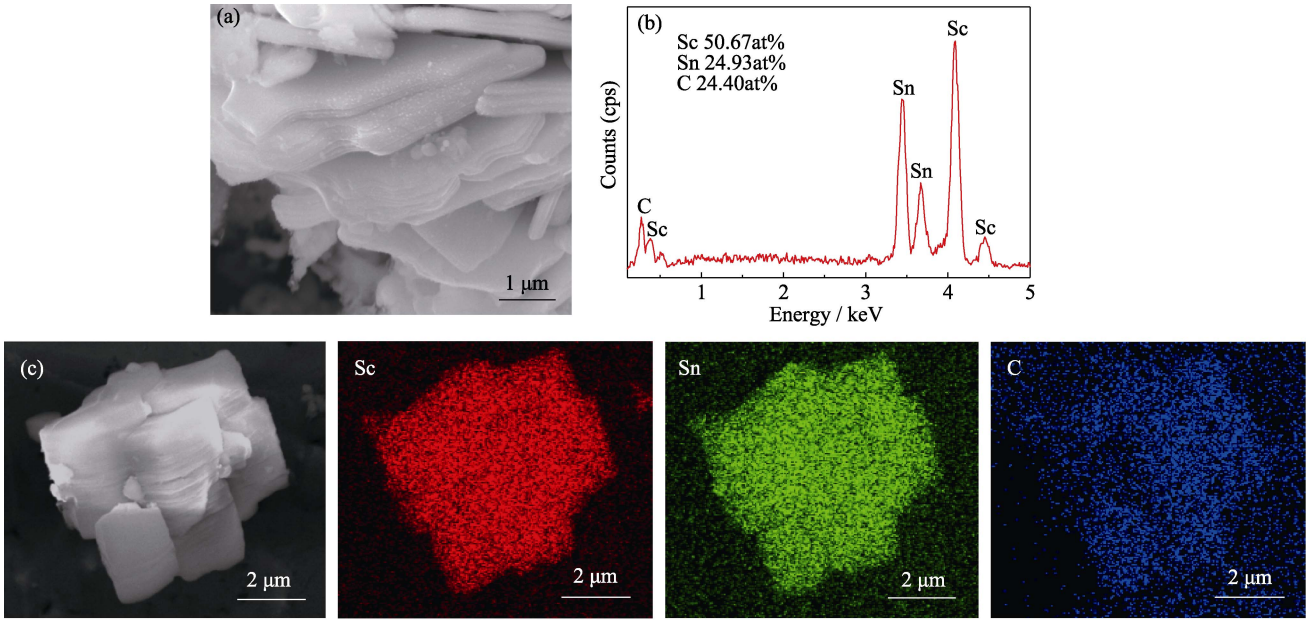

Fig. 3　(a) SEM image and (b) EDS analysis of Sc_2SnC, (c) elemental mappings of Sc, Sn and C elements

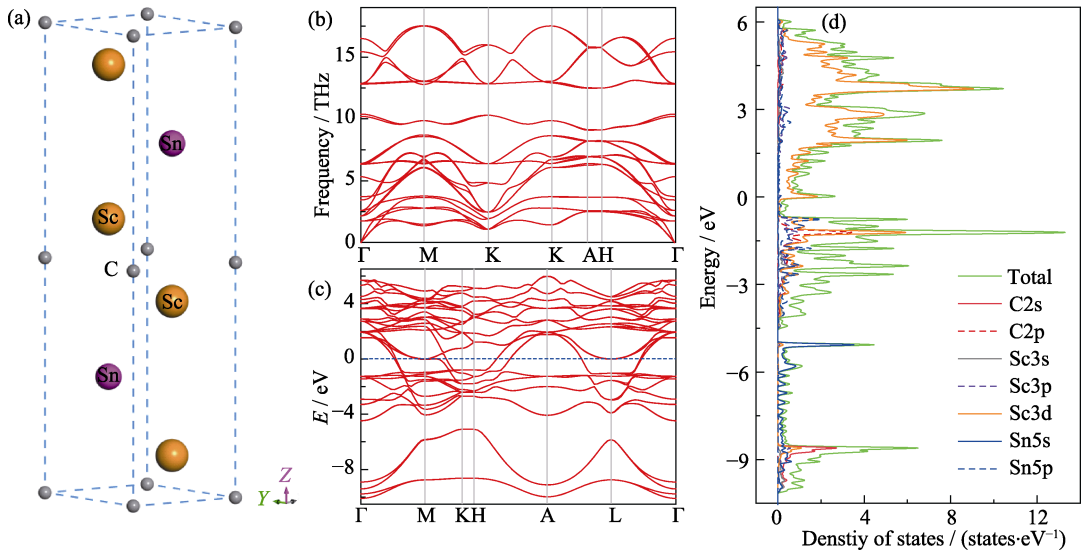

Fig. 4 (a) Crystal structure , (b) calculated phonon dispersion and (c) band structure of Sc_2SnC, and (d) projected density of Sc, Sn, and C atom states in the Sc_2SnC

calculated ΔH_{form} (Sc_2SnC) is –0.7167 eV, indicating the stability of Sc_2SnC phase. The lattice parameters, elastic constants and polycrystalline elastic modulus of Sc_2SnC, as well as for other Sn-containing MAX phases are listed in Table 2. From the DFT calculation result, *i.e.* a= 0.33686, c=1.46532 nm, is very close to experimental results. The mechanical stability of Sc_2SnC is justified from the Born stability criteria[36]: C_{11}>0, C_{11}-C_{12}>0, C_{44}>0, (C_{11}-C_{12})C_{33}-2C_{13}>0. Besides, the dynamical stability of Sc_2SnC can also be identified from the phonon dispersion curves in Fig. 4(b). The results performed by theoretical calculations are consistent with experiments. However, compared with other MAX phases (listed in Table 2), it is found that they have lower values of elastic constants (*i.e.* C_{11}, C_{33}, C_{44}, and C_{66}).

The relative small value of C_{33} indicates that the compound is more compressible along the c-axis compared to other studied compounds; while low C_{44} indicates being subject to shear deformation along $[11\bar{2}0]$ (0001); and small C_{66} probably means lower resistance to shear in the <110> direction[20,35,37]. The low shear deformation of Sc_2SnC is also reflected from shear modulus G, which represents the resistance to shape change of the polycrystalline material[38]. The calculated value of G/B >0.5 indicates that the phase is brittle in nature following Pugh's criterion. Furthermore, the obtained value of v (0.238) for Sc_2SnC shows that it locates at the boundary between covalent and ionic materials. The calculated band structure of Sc_2SnC and the projected density of states (DOS) of Sc, Sn, and C atoms with k-points are shown in Fig. 4(c, d), respectively. Similar to other MAX phases and MAX phase-like compounds, Sc_2SnC exhibits metallic nature, and the overlapping between valence and conduction bands across the Fermi level also reveals the presence of metallic bonding, which can be treated as the origin of the quasi-ductility of Sc_2SnC (Fig. 4(c)). From Fig. 4(d), it can be observed that the Sc-3d electrons are mainly contributing to the DOS at the Fermi level, and should be involved in the conduction properties, while the minor contributions come from Sn5p electrons.

Table 2 Theoretically predicted Lattice parameters (nm), calculated elastic constants, C_{ij} (GPa), bulk modulus, B (GPa), shear modulus, G (GPa), and Young's modulus, E (GPa), Pugh ratio, G/B, and Poisson ratio, v, of different compounds

Compound	a/nm	c/nm	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B	G	E	G/B	v	Ref.
Sc_2SnC	0.3368	1.4653	197	63	47	182	67	53	100	63	157	0.630	0.238	This work
V_2SnC	0.3134	1.2943	336	126	122	304	85	105	190	95	244	0.500	0.286	[35]
Ti_2SnC	0.3136	1.3641	337	86	102	329	169	126	176	138	328	0.784	0.188	[39]
Zr_2SnC	0.3352	1.4681	269	80	107	290	148	94	157	110	368	0.700	0.215	[39]
Hf_2SnC	0.3308	1.4450	330	54	126	292	167	138	173	132	316	0.763	0.195	[39]
Nb_2SnC	0.3244	1.3754	341	106	169	321	183	118	209	126	314	0.603	0.250	[39]

3 Conclusions

In conclusion, a new Sc_2SnC MAX phase was successfully synthesized by molten salt method for the first time. The XRD data of Sc_2SnC is useful for further phase identification and structure analysis, and Sc_2SnC exhibits a typical laminar microstructure similar to other MAX phases. The first-principle calculations were employed to further study structure stability of Sc_2SnC MAX phase, and the results show that Sc_2SnC is metallic in nature where the contribution from Sc-3d states dominates the electronic conductivity at the Fermi level. This work implies the great potential of the ternary rare-earth metal carbide $Re_{n+1}SnC_n$ (Re=Sc, Y, La-Nd, n=1) family waiting for further explore. More importantly, the introduction of rare earth elements can give the special properties of MAX phases, and can be used as a precursor material for preparing rare-earth MXenes.

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熔盐法合成纳米层状 Sc_2SnC MAX 相

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摘 要: MAX 相是一类兼具金属和陶瓷特性的三元层状材料, 也是合成二维 MXenes 的前驱体材料。理论预测稳定的三元层状 MAX 相材料约有 600 余种, 目前实验合成的三元层状 MAX 相材料已有 80 余种, 但 M 位主要为前过渡族金属, 而对 M 为稀土元素的三元 MAX 相鲜有报道。本研究以 Sc、Sn, 和 C 元素粉为原料, 通过熔盐法合成了 M 位为稀土元素 Sc 的全新 Sc_2SnC MAX 相材料。结合 X 射线衍射、扫描电子显微镜和 X 射线能谱等分析手段, 确认 Sc_2SnC MAX 的相组成和微观结构。并通过密度泛函理论计算了 Sc_2SnC MAX 相的结构稳定性、晶格参数、力学和电子性质, 理论计算结果表明 Sc_2SnC 热力学稳定, Sc-3d 电子在费米能级上占主导地位, MAX 相呈金属性质。

关 键 词: MAX 相; 纳米层状; 钪; 密度泛函理论计算

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