Molten Salt Synthesis of Nanolaminated Sc$_2$SnC 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$_2$SnC MAX phase via molten salt method. Phase composition and microstructure of Sc$_2$SnC 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$_2$SnC were investigated via density functional theory. The theoretical results show that Sc$_2$SnC is thermodynamically stable, and the Sc$_2$SnC 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$_{n+1}$Sc$_n$C ($Re=Sc$, 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$_2$InC 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$_2$InC 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$_2$CT$_2$ ($T=F$, OH) MXenes can be promising candidate materials for the next generation electronic devices[21]. Kuchida, et al[22] focused on non-transition metal M$_2$AX compounds which embody Sc, Y, and Lu atoms in M site, however, only polycrystalline sample of Lu$_2$SnC was reported. As a result, the study of new MAX phases taking Sc as M site element is an...
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\(^\text{[23]}\). Some MAX phases (e.g. Ti\(_3\)SiC\(_2\), Ti\(_3\)AlC\(_2\), V\(_2\)AlC, Cr\(_2\)AlC) have been synthesized by molten salt method\(^\text{[24-28]}\). In the present work, we synthesized a MAX phase of Sc\(_2\)SnC 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\(_2\)SnC 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)\(^\text{[16]}\). 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 °C for 3 h at heating rate of 5 °C/min under argon atmosphere, respectively. After the reaction was finished, the product was washed, filtered and dried at 40 °C 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\(_\alpha\) 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\(^\text{[29-30]}\), using the generalized gradient approximation (GGA) as implemented in the Perdew-Breke-Ernzerhof (PBE) functional\(^\text{[31-32]}\). Phonon calculations were carried out to evaluate the dynamical stability using the finite displacement approach, as implemented in CASTEP\(^\text{[33-34]}\). The equation \(E = (E_{\text{broken}} - E_{\text{bulk}})/S\)\(^\text{[13]}\) was adopted to calculate the cleavage energy \(E\), where \(E_{\text{broken}}\) and \(E_{\text{bulk}}\) 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\(_2\)SnC was by Total Pattern Solution (TOPAS-Academic V6) software.

2 Results and discussion

2.1 Phase analysis of the Sc\(_2\)SnC

Fig. 1(a) shows the XRD pattern of as-prepared powders synthesized at 1000 °C 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\(_2\)SnC is synthesized (also with minor amount of Sn metal as by-product). In comparison with experimental result, the simulated XRD pattern of Sc\(_2\)SnC 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\(_2\)SnC.

![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\(_2\)SnC](image)
XRD pattern is important for phase identification and structure analysis. Because no XRD pattern of Sc₂SnC was available in previous literatures, the Rietveld refinement of powder XRD pattern of Sc₂SnC was conducted. As shown in Fig. 2, the blue crosses represent the experimental diffraction profile (the Sn metal was removed by FeCl₃ solution), while the red solid line denotes the theoretical pattern. The theoretical Bragg diffraction positions of Sc₂SnC 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 Sc₂SnC is $P\overline{6}_3/mmc$ (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 V₂SnC in the previous report[35]. The atomic positions of Sc₂SnC determined from the Rietveld refinement are listed in Table 1.

### 2.2 Microstructural of the Sc₂SnC

It is well known that MAX phases crystallize in hexagonal structures and their grains are generally layered hexagons in morphology[1]. To confirm that Sc₂SnC has a similar microstructure, the microstructure of as-prepared powder was observed by SEM. It can be seen from Fig. 3(a) that Sc₂SnC 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 Sc₂SnC is experimentally synthesized.

### 2.3 DFT results

The structural analysis of Sc₂SnC phase was carried out via DFT calculations. Fig. 4(a) shows the ternary-layered carbide crystal structure of Sc₂SnC; and the

| 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 | 6m2      | 2d             |
| X    | C       | 0    | 0    | 0     | 3m       | 2a             |

Fig. 2 Comparison between experimental (blue line) and calculated XRD (red line) pattern of Sc₂SnC.

Table 1 Atomic positions in Sc₂SnC determined from the Rietveld refinement

Fig. 3 (a) SEM image and (b) EDS analysis of Sc₂SnC, (c) elemental mappings of Sc, Sn and C elements

calculated $\Delta H_{\text{form}}$ (Sc$_2$SnC) is $-0.7167$ eV, indicating the stability of Sc$_2$SnC phase. The lattice parameters, elastic constants and polycrystalline elastic modulus of Sc$_2$SnC, as well as for other Sn-containing MAX phases are listed in Table 2. From the DFT calculation result, i.e. $a=0.3368$, $c=1.4653$ nm, is very close to experimental results. The mechanical stability of Sc$_2$SnC 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$_2$SnC 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 $[11\overline{2}0]$ (0001); and small $C_{66}$ probably means lower resistance to shear in the $<110>$ direction$^{[20,35,37]}$. The low shear deformation of Sc$_2$SnC 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 $\nu$ (0.238) for Sc$_2$SnC shows that it locates at the boundary between covalent and ionic materials. The calculated band structure of Sc$_2$SnC 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$_2$SnC 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$_2$SnC (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, $\nu$, of different compounds

| Compound | $a$/nm | $c$/nm | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{33}$ | $C_{44}$ | $C_{66}$ | $B$ (GPa) | $G$ (GPa) | $E$ (GPa) | $G/B$ | $\nu$ | Ref. |
|----------|--------|--------|----------|----------|----------|----------|----------|----------|-----------|-----------|-----------|--------|-------|------|
| Sc$_2$SnC | 0.3368 | 1.4653 | 197 | 63 | 47 | 182 | 67 | 53 | 100 | 63 | 157 | 0.630 | 0.238 | This work |
| V$_2$SnC  | 0.3134 | 1.2943 | 336 | 126 | 122 | 304 | 85 | 105 | 190 | 95 | 244 | 0.500 | 0.286 | [35] |
| Ti$_2$SnC | 0.3136 | 1.3641 | 337 | 86 | 102 | 329 | 169 | 126 | 176 | 138 | 328 | 0.784 | 0.188 | [39] |
| Zr$_2$SnC | 0.3352 | 1.4681 | 269 | 80 | 107 | 290 | 148 | 94 | 157 | 110 | 368 | 0.700 | 0.215 | [39] |
| Hf$_2$SnC | 0.3308 | 1.4450 | 330 | 54 | 126 | 292 | 167 | 138 | 173 | 132 | 316 | 0.763 | 0.195 | [39] |
| Nb$_2$SnC | 0.3244 | 1.3754 | 341 | 106 | 169 | 321 | 183 | 118 | 209 | 126 | 314 | 0.603 | 0.250 | [39] |
3 Conclusions

In conclusion, a new Sc₂SnC MAX phase was successfully synthesized by molten salt method for the first time. The XRD data of Sc₂SnC is useful for further phase identification and structure analysis, and Sc₂SnC exhibits a typical laminar microstructure similar to other MAX phases. The first-principle calculations were employed to further study structure stability of Sc₂SnC MAX phase, and the results show that Sc₂SnC 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 Reₙ₋₁SnCₙ₊₁ (Re=Sc, Y, La-Nd, n=1) family for the first 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$_2$SnC 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$_2$SnC 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$_2$SnC MAX 相的组成和微观结构。并通过密度泛函理论计算了 Sc$_2$SnC 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$_2$SnC 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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