

# Quaternary representative of the Cr<sub>2</sub>AlC-type structure in the Ti–Al–Ga–C system

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In the Ti–Al–C system, the Ti<sub>2</sub>AlC compound forms with a Cr<sub>2</sub>AlC-type structure, classified among the MAX phases. These materials are particularly promising due to their unique layered structure, which imparts a combination of metallic and ceramic properties. They offer excellent electrical and thermal conductivity, are relatively soft and easy to machine, resist thermal shocks and oxidation, present high thermal stability, and have a high melting point. Currently, over 150 compounds are known to belong to the MAX phase family, each one exhibiting distinct properties [1]. This diversity has driven researchers to explore new element combinations in the pursuit of materials with tailored characteristics. The formation of static mixtures of Al and Ga atoms has been observed in the Cr–Al–Ga–C and V–Al–Ga–C systems [2]. A continuous solid solution is known to form in the Ti–Al–Ga ternary system [3], which motivated us to further investigate this quaternary system.

Samples were synthesized using elemental powders of Ti, Al, and C, along with metallic Ga pieces. Two compositions were prepared: Ti<sub>50</sub>Al<sub>14</sub>Ga<sub>14</sub>C<sub>22</sub> and Ti<sub>50</sub>Al<sub>10</sub>Ga<sub>10</sub>C<sub>30</sub>. The synthesis was carried out in two stages. Stage 1 involved sintering in an induction furnace at 900°C for 10 minutes to prevent the presence of unreacted Ga. All processes were conducted in a glove box under an argon atmosphere. The sintered material was then ground using a ball mill to prepare for the next stage. Stage 2 involved spark plasma sintering (SPS). The temperature was monitored using a pyrometer. Initially, the samples were heated to 600°C and held for one minute. The Ti<sub>50</sub>Al<sub>14</sub>Ga<sub>14</sub>C<sub>22</sub> sample was then heated to 1200°C, while the Ti<sub>50</sub>Al<sub>10</sub>Ga<sub>10</sub>C<sub>30</sub> sample was heated to 1300°C, both at a rate of 10 K/min. Each sample was held at its respective peak temperature for 2 h under a pressure of 65 MPa. Finally, the samples were cooled to room temperature over a period of 30 minutes.

X-ray diffraction (XRD) revealed that both samples consisted of two phases: a primary phase with Cr<sub>2</sub>AlC-type structure and a secondary TiC phase. For the Ti<sub>50</sub>Al<sub>14</sub>Ga<sub>14</sub>C<sub>22</sub> sample, the primary phase constituted 97.4 wt.%, while TiC accounted for 2.6 wt.%. The Ti<sub>50</sub>Al<sub>10</sub>Ga<sub>10</sub>C<sub>30</sub> sample contained 85.2 wt.% of the primary phase and 14.8 wt.% TiC. The presence of these two phases was further confirmed by energy-dispersive X-ray spectroscopy (EDX), which also provided insights into the elemental composition, particularly the Al-to-Ga ratio. According to EDX data, the Ti<sub>50</sub>Al<sub>14</sub>Ga<sub>14</sub>C<sub>22</sub> sample had an approximate elemental ratio of Ti:Al:Ga:C = 50.9:12.7:9.4:27.0, while the Ti<sub>50</sub>Al<sub>10</sub>Ga<sub>10</sub>C<sub>30</sub> sample showed a ratio of 44.6:8.2:6.5:40.7. Although EDX is less accurate for quantifying carbon, due to its low sensitivity to light elements, the method still provides useful information about phase purity and compositional trends.

Crystallographic data for the samples are presented in Table 1.

**Table 1.** Crystallographic data of the compound with Cr<sub>2</sub>AlC-type structure (Pearson symbol *hP8*, space group *P6<sub>3</sub>/mmc*) for samples Ti<sub>50</sub>Al<sub>14</sub>Ga<sub>14</sub>C<sub>22</sub> and Ti<sub>50</sub>Al<sub>10</sub>Ga<sub>10</sub>C<sub>30</sub>

Sample		Ti <sub>50</sub> Al <sub>14</sub> Ga <sub>14</sub> C <sub>22</sub>				Ti <sub>50</sub> Al <sub>10</sub> Ga <sub>10</sub> C <sub>30</sub>			
Compound		Ti <sub>2</sub> Al <sub>0.39(1)</sub> Ga <sub>0.61(1)</sub> C				Ti <sub>2</sub> Al <sub>0.49(1)</sub> Ga <sub>0.51(1)</sub> C			
Cell parameters, Å		<i>a</i> = 3.06147(9), <i>c</i> = 13.4590(5)				<i>a</i> = 3.06259(7), <i>c</i> = 13.4906(4)			
Site	Wyckoff position	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> <sub>iso.</sub> , Å <sup>2</sup>	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> <sub>iso.</sub> , Å <sup>2</sup>
Ti	4 <i>f</i>	1/3	2/3	0.0848(3)	0.55(2)	1/3	2/3	0.0843(3)	0.58(2)
<i>M</i>	2 <i>c</i>	1/3	2/3	1/4	0.64(4)	1/3	2/3	1/4	0.67(4)
C	2 <i>a</i>	0	0	0	0.7	0	0	0	0.7
		<i>M</i> = 0.39(1)Al + 0.61(1)Ga				<i>M</i> = 0.49(1)Al + 0.51(1)Ga			

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