Evaluating the geometry of titanium (Ti_7) cluster in $TiCl_3$ medium

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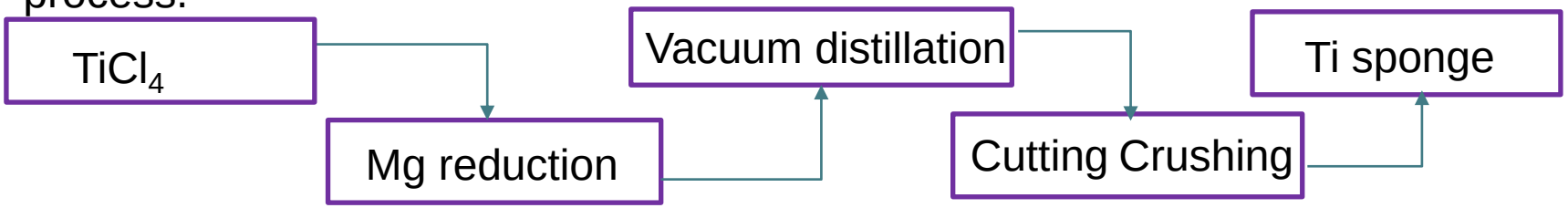
Introduction

- Significance of titanium: High strength-weight ratio, excellent corrosion resistance (thin protective oxide layer), low density and biocompatibility [1].



- Titanium can be produced commercially through thermochemical processes e.g. Kroll process.

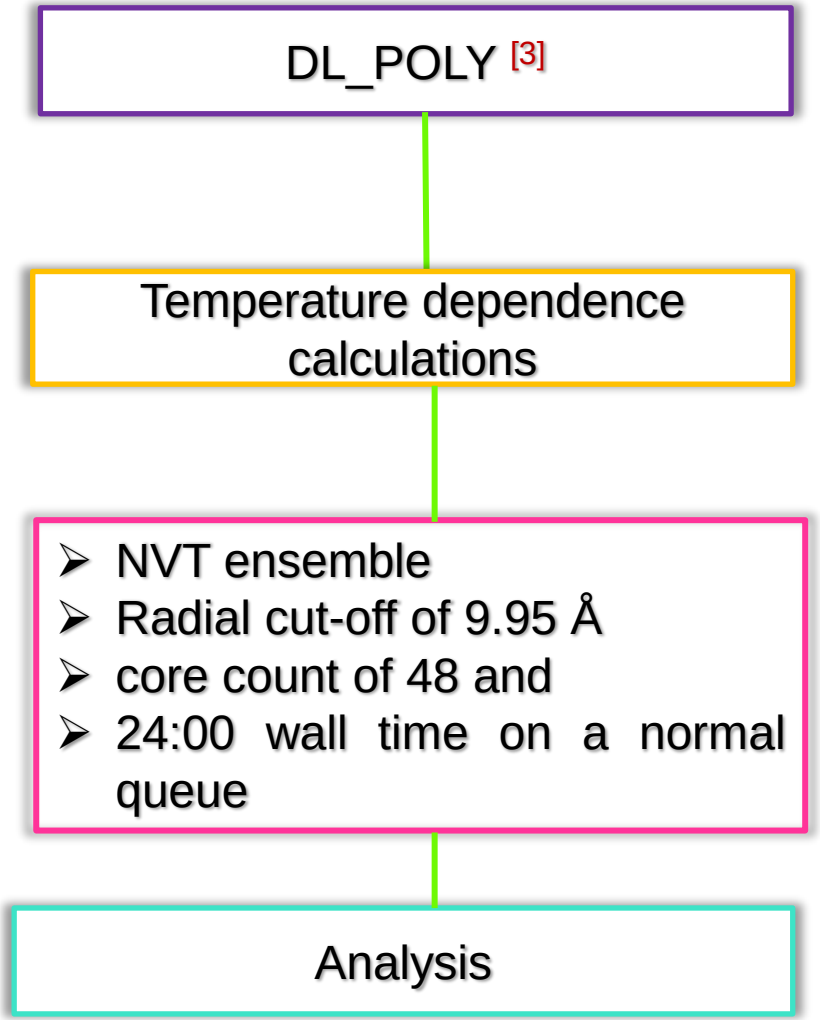


- However, this process occurs extremely fast, with the formed titanium deposits firmly adhering to the reactor[2].

- In this study we will use a computational modelling approach to understand the geometry of the cluster after interactions with $TiCl_3$ (P-31m) medium.

[1] Takeda O. and Okabe T.H., *Materials Transactions*, **47**, pp.1145, 2006.
[2] Noda T., *Journal of Metals*, **17**, pp. 25, 1965.

METHODOLOGY



[3] Todorov I.T. Smith W. Trachenko K. and Dove M.T., *Journal of Materials Chemistry,* **16**, pp. 1911, 2006.

Results

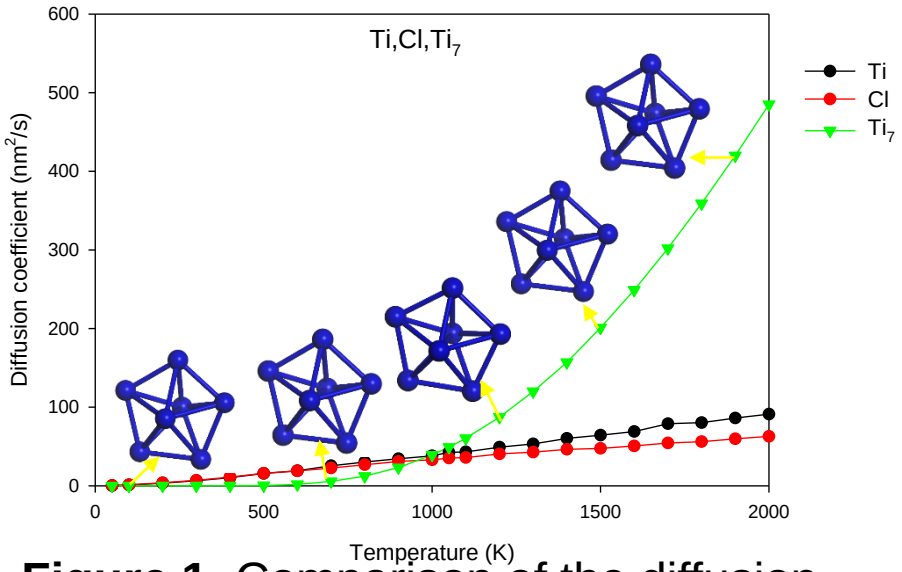


Figure 1. Comparison of the diffusion coefficient of Ti, Cl and Ti_7 in $Ti_7/TiCl_3$ (P-31m) medium.

The cluster diffuses faster at 1050 K – 2000 K.

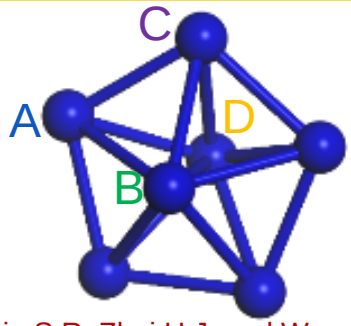


Table 1. The calculated Ti_7-Ti_7 bond length in the $Ti_7/TiCl_3$ system at different temperatures.

		Ti_7-Ti_7 bond length (Å)		
Bond site		A-B	B-D	A-C
Theor.[4]		2.59	2.51	2.60
Ground state		2.567	2.868	2.503
Calc.	50 K	2.484	2.715	2.446
	300 K	2.481	2.707	2.446
	600 K	2.473	2.764	2.421
	900 K	2.513	2.769	2.417
	1100 K	2.560	2.653	2.471
	1400 K	2.407	2.766	2.572
	1700 K	2.368	2.700	2.464
	2000 K	2.456	2.648	2.428

Elongation of Ti_7-Ti_7 bond along A-C from 2.503 Å at 50 K to 2.572 Å at 1400 K.

[4] Castro M. Liu S.R. Zhai H.J. and Wang L.S. *J. Chem. Phys*. **118**, pp. 2116, 2003.

Conclusion & Acknowledgements

- The DC results show that the cluster diffuses faster at high temperatures (1050 K – 2000 K)
- The cluster maintains its ground state pentagonal bipyramid geometry at the temperature range of 50 K – 2000 K.
- The results obtained in this study might provide more insight into the growth/evolution of titanium in $TiCl_3$ medium for titanium production processes.

NRF National Research Foundation

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