Role of N Diffusion Kinetics in Creating an Atomically Chemically Graded Ti/TiN Interface

J.VARALAKSHMI [A] PRINCE GOLLAPALLI [A] SATYESH KUMAR YADAV [A,B,]

[a] Department of Metallurgical and Materials Engineering, Indian Institute of Technology (IIT) Madras, Chennai 600036, India
[b] Center for Atomistic Modelling and Materials Design, Indian Institute of Technology (IIT) Madras, Chennai 600036, India

ABSTRACT

Recent calculations based on DFT suggest that it is thermodynamically favorable for N to diffuse across a sharp Ti/TiN interface from TiN to Ti [1]. Only migration of N atom across a sharp Ti/TiN interface is required to create the atomically chemical-graded interface, as a range of Ti-N stoichiometry could be achieved by migration of N without changing Ti position. On TiN side of the interface, Ti_6N_5, Ti_4N_3, Ti_3N_2 can form from rock salt TiN by forming ordered N vacancy. Similarly, on Ti side, N interstitials solid solution in Ti can form by intercalation of N. We explore the diffusion path of N migration from TiN to Ti and the rate of N diffusion. We calculate the diffusion coefficient of N in: 1) TiN, 2) Ti_6N_5, 3) Ti_4N_3, 4) Ti, 5) Ti-0.14N 6) Ti-0.2N, and 7) across the sharp Ti/TiN interface. We use DFT to calculate the barrier to diffusion of N along various possible paths and frequencies at the stable and transition states. Then, we calculate the diffusion coefficient within Arrhenius theory [2]. We show that the diffusion coefficient for N diffusion is slowest in TiN and fastest in Ti, while that across the interface is between TiN and Ti. Slowest diffusion of N in TiN leads to the formation of the chemically graded interface on annealing alone.

Keywords: Metal/ceramic interface; vacancy formation energy; interstitial formation energy; barrier energy; diffusion coefficient; Arrhenius theory density functional theory; nanoheterostructure

References

[1] Gollapalli, Prince & **Varalakshmi, J**. & Kishor, P.S.V.R.A. & Oza, Prajeet & Yadav, Satyesh. (2022). Atomically chemically graded Ti/TiN interface. Applied Surface Science. 597. 153637. 10.1016/j.apsusc.2022.153637.

[2] H. H. Wu and D. R. Trinkle, Phys. Rev. Lett. 107, 045504 (2011).