

Introduction

Multi-layer titanium nitride/titanium aluminium nitride film growth was simulated by means of kinetic Monte Carlo code NASCAM [1]. Film growth was simulated for different number of bi-layers TiN/TiAlN, with the number of bi-layers equals from 5 to 100. Results of the simulation were compared to experimental data [2]. It was shown that interfaces between individual layers make a significant contribution to a total thermal resistivity of the multi layer film.

Calculation of the thermal conductivity of simulated multi-layer film was conducted in two steps. Firstly, the thermal conductivity of the single layer was calculated by using Landauer relation based on effective medium theory [3]:

$$k = \left[k_p(3n_p - 1) + k_0(2 - 3n_p) + \left\{ [k_p(3n_p - 1) + k_0(2 - 3n_p)]^2 + 8k_0k_p \right\}^{1/2} \right] / 4 \quad (1)$$

where n_p and k_p are porosity of the film and thermal conductivity of material which fills the pores, normally it equals to 0. Interesting, that the relation is the same as Bruggeman's relation for effective dielectric constant.

Secondly, the thermal conductivity of the whole stack was calculated the following equation:

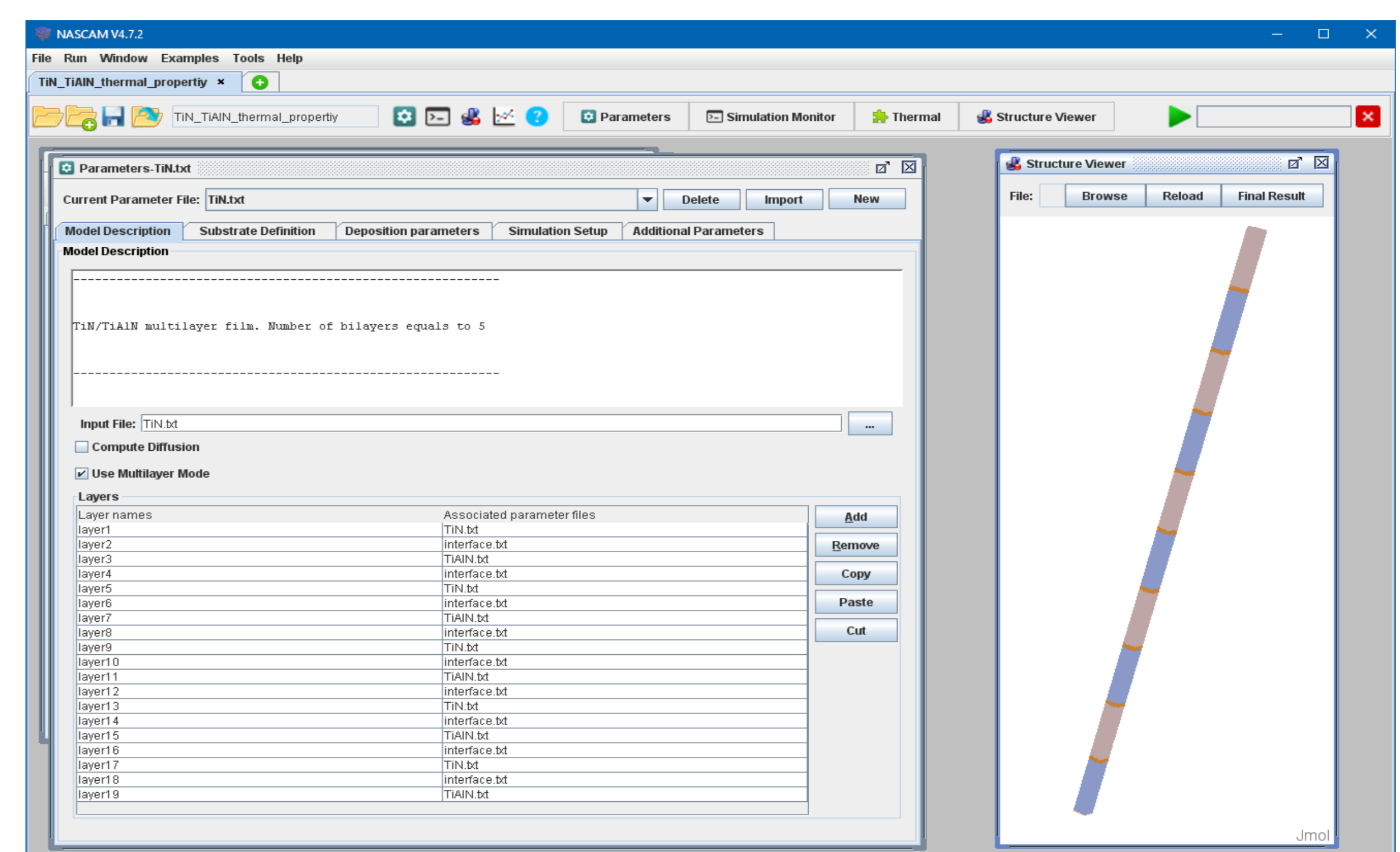
$$\frac{1}{k} = \sum_{i=1}^N \frac{l_i/l}{k_i} + \sum_{j=1}^{N-1} r_j, \quad (2)$$

where k_i is a thermal conductivity of a sub-layer "i", l_i is a thickness of the sub-layer "i", l is the total thickness of the layer, and N is the number of sub-layers and r_j are thermal resistivities of the interfaces between each TiN and TiAlN layers.

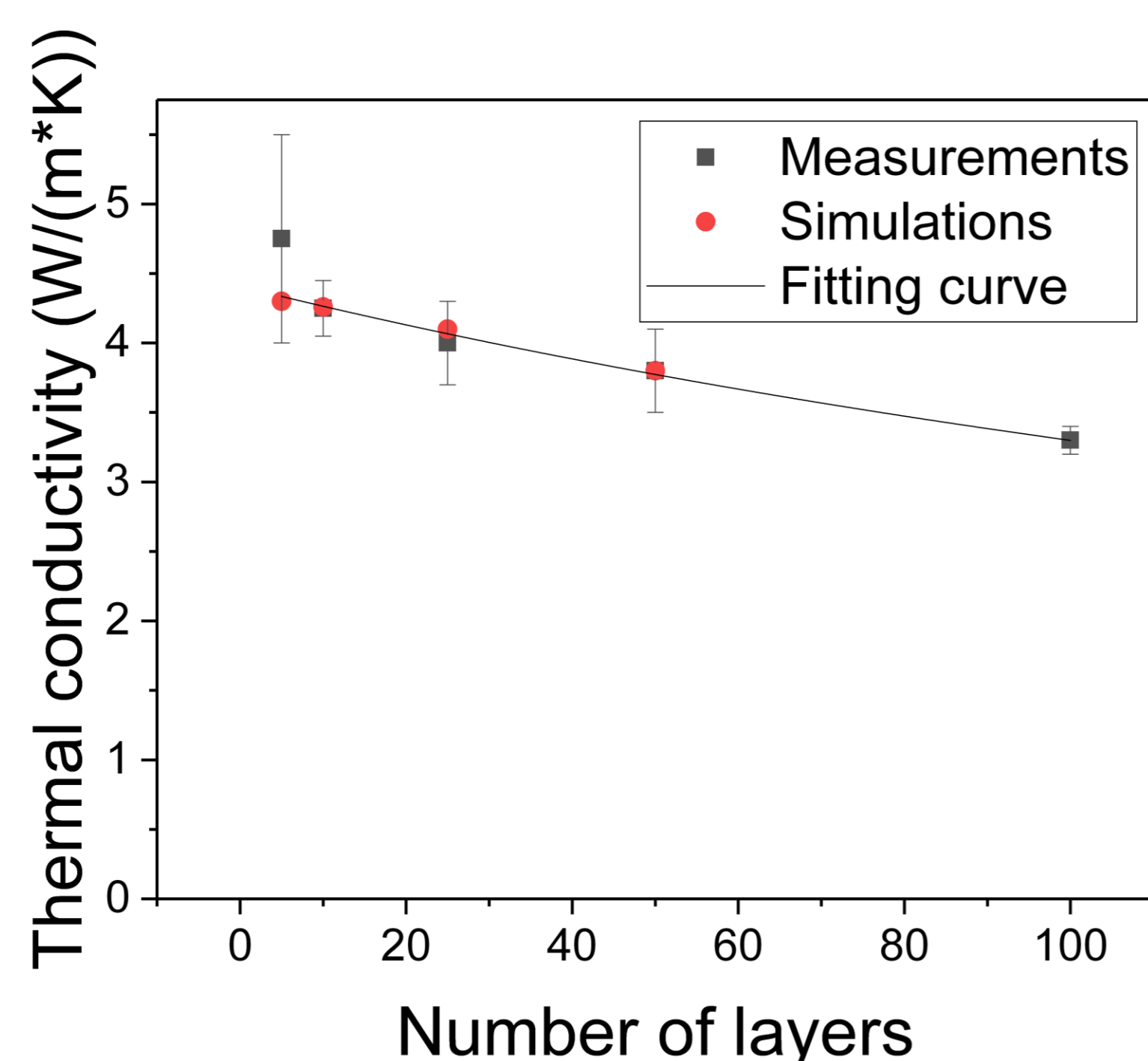
Firstly, it is necessary to setup NASCAM simulation for cases of multilayer deposition. To simulate such a film one has to simulate deposition $N = 4*n-1$ single layers. This number is easy to understand if one takes into account that the structure of the film is as follow:

TiN/Interface/TiAlN/interface/
TiN/interface/TiAlN/interface/
.../
TiN/interface/TiAlN/interface/
TiN/interface/TiAlN/

Therefore, for each bilayer it is necessary to simulate 4 single layers.



Simulation of deposition of 5 bilayers of TiN/TiAlN.



Experimental values of thermal conductivity of TiN/TiAlN multi layer film and values simulated by Thermal plugin and calculated by Eq. 2

Conclusions

The growth of multi layer TiN/TiAlN film was simulated by kinetic Monte Carlo code NASCAM. Then the thermal conductivity of the coating was evaluated both analytically and by analysis of simulated film. A good agreement with experimental data was obtained.

It was shown that when dealing with multi layer coating it is necessary to take into account the thermal resistivity of the interfaces between individual layers, which contribute significantly to the overall thermal resistance of the coating.

References

- [1] <https://www.unamur.be/sciences/physique/ur/larn/logiciels/nascam>
- [2] M.K. Samani et al, Thermal conductivity of titanium nitride/titanium aluminium nitride multilayer coatings deposited by lateral rotating cathode arc, Thin Solid Films 578 (2015) 133–138).
- [3] R. Landauer, The electrical resistance of binary metallic mixtures, J. Appl. Phys. 23, 779-784, 1952