



Self-propagating combustion Simulation of sputter-deposited Nano-Energetic Multilayer Films

Anran Shi, Wei Zhang, Ruiqi Shen *

Department of Applied Chemistry, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China
E-mail: arshi@njjust.edu.cn

Introduction

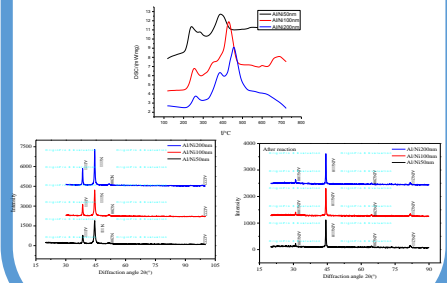
Nano reactivity multilayers films (nRMFs) are 2-Dimension nano-energetic materials that is wildly used in energetic chips, but it was found that the released heat of RMFs is less than their theoretical value, and the released heat depended on the thickness of reactants or layers. The interface chemical pre-reactions between two boundary layers was considered to be decreasing reason of released heat. The dependence of released heat on the thickness of layer will be researched to find the interface reaction mechanism of Al/Ni, Al/Ti multilayer films by DSC and XRD.

Stoichiometric nRMFs

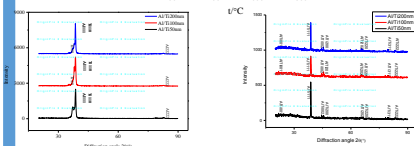
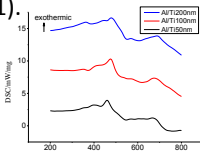
The stoichiometric reactants are required to design high exothermal NEML. The ratio or thicknesses of two reactants can be calculated in Equ

$$\frac{H_1}{H_2} = \frac{m_1 \rho_2}{m_2 \rho_1} = \lambda_{12} \frac{M_1 \rho_2}{M_2 \rho_1}$$

Reactivity of Nano RMFs



Before reaction, the compositions of Al/Ni nRMFs include Al(111), Al(222), Ni(111), Ni(200), but the diffraction peak of Al_xNi_y (AlNi(110)) does not confirmed, since it overlaps with the diffraction peak of Ni(111). After reaction, the compositions are AlNi(100), AlNi(110), AlNi(200), AlNi(211).



XRD analyzed results of initial Al/Ni nRMFs are Al(111), Al(222), Ti(100), Ti(110), but because AlTi(111) peak overlaps Al(111) peak, Al_xTi_y does not been confirmed. After reaction, XRD analyzed results of reacted Al/Ti nRMFs show that the compositions are AlTi(001), AlTi(111), AlTi(002), AlTi(200), AlTi(202), AlTi(220), AlTi(311), AlTi(222), in which AlTi(111) is main reacted product.

Conclusion

Some chemical pre-reactions at interface of reactivity multilayer films (RMFs) are avoided, that will develop a pre-reaction layer between two boundary surfaces of reactants and let the reaction heat of RMFs decrease. The XRD analyzed results of Al/Ni, Al/Ti shown that there is no obvious evidence of pre-reaction layer, such as Al_xNi_y, but some cases are overlapping XRD peaks of reactants and pre-reaction products. That is to say the possible pre-reaction layer is existed. DSC analyzed supported the view of pre-reaction. The heat of reaction depends on the thickness of reactant layers, in which the thinner reactant layer, the less reaction heat of RMFs. A simple equation is derived to calculate the thickness of pre-reaction by the experimental data of RMFs reaction heat