

On the Mechanism of Nitrogen Diffusion in Nitrides

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ABSTRACT

We have developed a model explaining and predicting generation of a temporal electric potential during nitridation of a single metal pellet. The model takes into account the kinetics of defects formation and assumes that the rate of the chemical reaction can be described by the shrinking-core process.

As in oxygen combustion, preliminary calculation results have shown that the maximum of the surface electric potential is attained before the temperature and the surface nitrogen concentration have reached their maximums but after the maximum of nitridation has appeared. In contrast to oxidation, nitrogen adsorption rate constants (the activation energy and pre-exponent) have negligible effect on the surface potential form and amplitude. At the ignition limit, the rate of nitridation is proportional to the power of $-1/2$ for the ambient nitrogen pressure for the proposed scheme of defects formation. Metal vacancies and electron holes are the main charged defects in nitrides during nitrogen combustion. The nitride formation is limited by transfer of metal vacancies in nitride.

Key words: *nitridation, single metal pellet, transient surface potential, defects formation, metal vacancies and electron holes.*