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Nucleation and growth on defect sites: experiment–theory comparison for Pd/MgO(001)

J A Venables[1,2,5], **L Giordano**[3] **and J H Harding**[4]

[1] Department of Physics and Astronomy, Arizona State University, Tempe, AZ 85287, USA
[2] School of Science and Technology, University of Sussex, Brighton BN1 9QH, UK
[3] Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, 53-20135 Milano, Italy
[4] Department of Engineering Materials, University of Sheffield, Sheffield S1 3JD, UK

E-mail: john.venables@asu.edu

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Abstract

It is well established that nucleation of metal clusters on oxide and halide surfaces is typically dominated by defect sites. Rate equation models of defect nucleation have been developed and applied to these systems. By comparing the models with nucleation density experiments, energies for defect trapping, adsorption, surface diffusion and pair binding have been deduced in favourable cases, notably for Pd deposited on Ar-cleaved MgO(001). However, the defects responsible remain largely unknown. More recently, several types of *ab initio* calculation have been presented of these energies for Pd and related metals on MgO(001) containing several types of surface defect; these calculated values are surveyed, and some are widely divergent. New rate equation nucleation density predictions are presented using the calculated values. Some calculations, for some defect types, are much closer to experiment than others; the singly charged F_s^+ centre and the neutral divacancy emerge as candidate defects. In these two cases, the Pd/MgO(001) nucleation density predictions agree well with experiment, and the corresponding surface defects deserve to be taken seriously. Energy and entropy values are discussed in the light of differences in calculated charge redistribution between the metal atoms, clusters and (charged) surface defects, and (assumed or calculated) cluster geometries.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Thin metal clusters supported on oxide surfaces have many practical applications due to their catalytic, magnetic and electric properties; experiment and theory have given rise to a large

[5] Author to whom any correspondence should be addressed.

