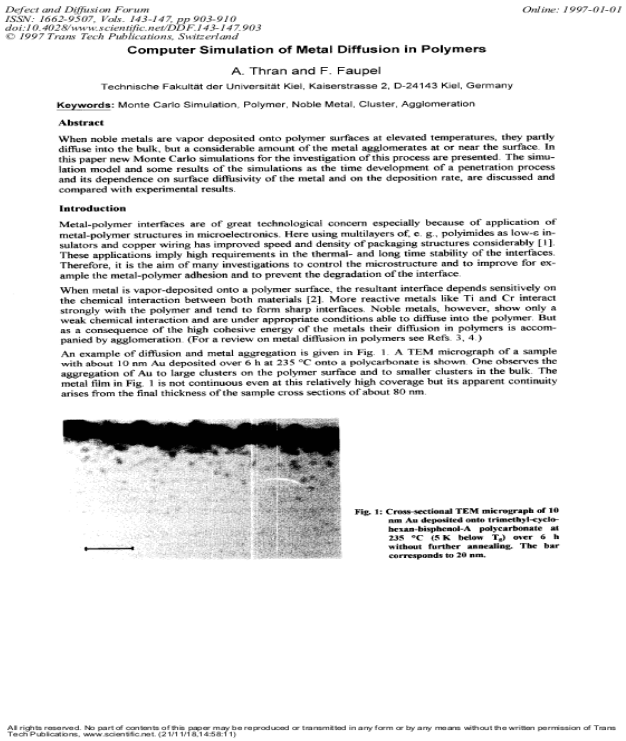
Computer Simulation Of Polymers



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Computer Simulation of Metal Diffusion in Polymers

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Abstract

When noble metals are vapor deposited onto polymer surfaces at elevated temperatures, they partly diffuse into the bulk, but a considerable amount of the metal agglomerates at or near the surface. In this paper new Monte Carlo simulations for the investigation of this process are presented. The simulation model and some results of the simulations as the time development of a penetration process and its dependence on surface diffusivity of the metal and on the deposition rate, are discussed and compared with experimental results.

Introduction

Metal-polymer interfaces are of great technological concern especially because of application of metal-polymer structures in microelectronics. Here using multilayers of, e. g., polyimides as low-ε insulators and copper wiring has improved speed and density of packaging structures considerably [1]. These applications imply high requirements in the thermal- and long time stability of the interfaces. Therefore, it is the aim of many investigations to control the microstructure and to improve for example the metal-polymer adhesion and to prevent the degradation of the interface.

When metal is vapor-deposited onto a polymer surface, the resultant interface depends sensitively on the chemical interaction between both materials [2]. More reactive metals like Ti and Cr interact strongly with the polymer and tend to form sharp interfaces. Noble metals, however, show only a weak chemical interaction and are under appropriate conditions able to diffuse into the polymer. But as a consequence of the high cohesive energy of the metals their diffusion in polymers is accompanied by agglomeration. (For a review on metal diffusion in polymers see Refs. 3, 4.)

An example of diffusion and metal aggregation is given in Fig. 1. A TEM micrograph of a sample with about 10 nm Au deposited over 6 h at 235 °C onto a polycarbonate is shown. One observes the aggregation of Au to large clusters on the polymer surface and to smaller clusters in the bulk. The metal film in Fig. 1 is not continuous even at this relatively high coverage but its apparent continuity arises from the final thickness of the sample cross sections of about 80 nm.

Fig. 1: Cross-sectional TEM micrograph of 10 nm Au deposited onto trimethyl-cyclo-hexan-bisphenol-A polycarbonate at 235 °C (5 K below T_g) over 6 h without further annealing. The bar corresponds to 20 nm.

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