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Structure of molybdenum-phosphate glasses by X-ray photoelectron spectroscopy (XPS)

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Abstract

Highly-concentrated molybdenum-phosphate glasses with analyzed compositions of Mo greater than 0.65 have been studied by X-ray photoelectron spectroscopy (XPS) and magnetization measurements. 1 eV shifts in the binding energies of P2p, P2s, Mo3d, and Mo3p from their respective values in P_2O_5 and MoO_3 can be accounted for by changes in the next nearest neighbor environment of the P and Mo atoms upon the mixing of the two glass formers. The O1s spectrum is deconvoluted into two peaks with the lower-energy peak being associated with the oxygen atoms of the non-bridging P=O structure as well as from various M–O bonds and the higher-energy peak with the bridging oxygen atoms of the P–O–P structure. From the amount of Mo^{6+} reduced to Mo^{5+}, as determined from the magnetization results, the variations in the areas of these O1s peaks are discussed in terms of an existing structural model based on this binary glass being composed of a mixture of the structural groupings which occur in the crystalline phases of the MoO_3:P_2O_5 system.

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1. Introduction

Studies of oxide glasses containing large concentrations of transition-metal (TM) oxides continue to be of interest because of their semiconducting properties and potential applications [1–4]. The electrical conduction in these glasses results from electron hopping between two TM ions having different valence states. However, a more detailed modeling of the conduction process is limited because of numerous material factors including the type and concentration of the TM ion, the number of valence states associated with the TM ion, the glass preparation conditions, and the microstructures within the glass matrix. Thus, information on the structure of a glass is imperative for further elucidating our understanding of the glass properties.

X-ray photoelectron spectroscopy (XPS) has proven to be not only a powerful tool for investigating the electronic structure in solids, but also the bonding and hence the local structure [5–7]. When a specimen is irradiated by a beam of X-rays, photoelectrons can be ejected from its atoms with kinetic energies E_k. From the conservation of energy, the

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