Self-consistent diffraction stress analysis for estimating stress and composition of alloy films

T. Harumoto, J. Shi, Y. Nakamura

Department of Materials Science and Engineering, Tokyo Institute of Technology, Tokyo 152-8552, Japan

harumoto.t.aa@m.titech.ac.jp

In the case of alloy films and multilayers, measure of composition may be hard, since the volume of film is far less than that of substrate. Therefore, the surface sensitive measurements, such as X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES), are employed frequently. Alterative way is the chemical etching of film followed by the concentration analysis of the aqueous solution. However, all these methods are destructive and can be performed only under ex-situ condition. Also, diffraction stress analysis of alloy films may be difficult, since the composition is required for estimating the diffraction elastic constants.

Considering the situation described above, we proposed the self-consistent diffraction stress analysis method for analysing composition and stress (Fig. 1) [1]. This method is based on the strain-free lattice parameter, which is generally treated as a by-product of diffraction stress analysis and receives less attention. However, we here tried to utilize it, since it contains the information of composition. The main concept of the proposed method is the feedback of the strain-free lattice parameter in the form of composition. Due to the feedback, the diffraction stress analysis can be performed even when the exact composition is unknown. After the convergence of feedback calculation, the final results are composition and stress; they have self-consistency.

The validity of this analysis method was experimentally confirmed using example specimens of (111) fibre-textured palladium cobalt (PdCo) alloy films with different composition. Note that PdCo alloy films are expected as the next generation magnetism-based hydrogen sensor, since they absorb hydrogen and show both perpendicular magnetic anisotropy and large magnetostriction constant [2-4]. The lattice spacings measured at the different tilt angles are analysed using the proposed method. It was revealed that the self-consistent calculation converged well and the resultant composition is in a good agreement with the result of AES. The difference of composition is 1 at.%, even though this method only provides the estimated composition from the strain-free lattice parameter. The resultant stress also shows an agreement with one of the conventional diffraction stress analysis.

The proposed self-consistent method is suitable for cases, such as *in-situ* measurement, where the measure of composition is difficult. This method expands the applicability of diffraction stress analysis.

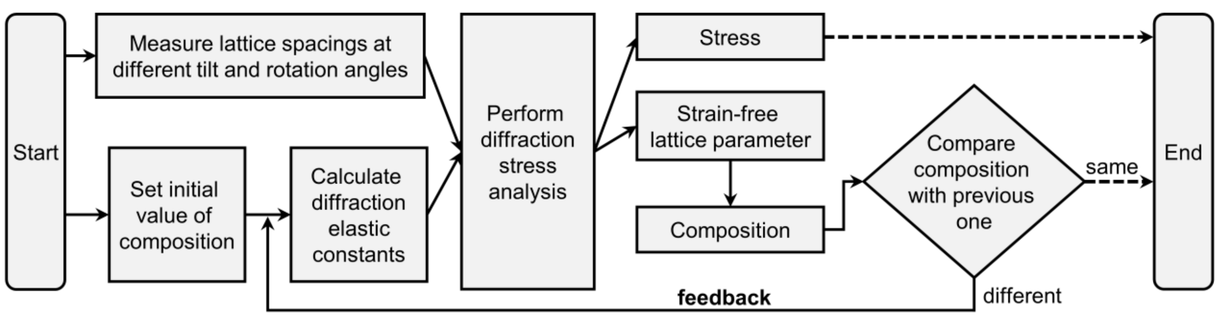

Figure 1. Concept of self-consistent diffraction stress analysis method for estimating stress and composition of alloy films.

[1] Harumoto, T., Shi, J. & Nakamura, Y. (2020). *Mater. Trans.* **61**, 1922.

[2] Akamaru, S., Matsumoto, T., Hara, M., Nishimura, K., Nunomura, N. & Matsuyama, M. (2013). *J. Alloy. Compd.* **580**, S102.

[3] Chang, P.C., Chen, Y.C., Hsu, C.C., Mudinepalli, V.R., Chiu, H.C. & Lin, W.C. (2017). *J. Alloy. Compd.* **710**, 37.

[4] Harumoto, T., Shi, J. & Nakamura, Y. (2019). *J. Appl. Phys.* **126**, 083906.

Keywords: diffraction stress analysis; strain-free lattice parameter; composition; film; texture

This research is supported by Grants-in-Aid for Scientific Research Kakenhi (grant No. 18K14137) from Japan Society for the Promotion of Science (JSPS).