Structures in Mo-Ru-Si System by Powder and Anomal X-Ray Diffraction

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$MoSi_2$ attracted extensive interest during the last years because of its great potential for new high temperature structural materials. In order to improve $MoSi_2$ performance against "pest" phenomenon and glass corrosion at 1350°C additions of ruthenium metals have been made. This original way led us to investigate the Mo-Ru-Si ternary system that revealed the existence of five new phases noted α ($Mo_{15}Ru_{35}Si_{50}$), β($Mo_{26}Ru_{47}Si_{27}$), γ($Mo_{41}Ru_{41}Si_{18}$), δ($Mo_{15}Ru_{50}Si_{35}$), and σ($Mo_{60}Ru_{30}Si_{30}$). The phases α and σ are isotypes of the FeSi and FeCr structures respectively. The structures of the β and γ phases were determined ab-initio from synchrotron X-ray powder diffraction (XRPD) data. All of these phases are partially disorder with statistical occupancy of sites by the various metallic atoms. In order to increase the contrast between Mo and Ru and to obtain a crystallographic composition, X-Ray powder patterns were performed at the Mo-K threshold (20 keV) so as to use the anomal effect. Therefore, multi refinement pattern using two wave lengths (one near the Mo Threshold, the other out) has been performed. Subsequently, an assessment of the site occupancy rates allowed to specify the distribution of the Mo (Z = 42) and Ru (Z = 44) atoms. Extension of the stability domain of β phase $Mo_{4+x}Ru_{9-x}Si_5$ ($0 \leq x \leq 1$) is understood on the basis of the XRPD results and electronic properties calculation (KKR method) as a function of the composition [1].

[1] Littner A., François M., Tobola J., Elkaim E., Malaman B., Vilasi M., Intermetallics, 2005, in press.

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