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First-principles study of the Hume-Rothery electron concentration rule in Al-Cu-(Fe,Ru)-Si 1/1-cubic approximants[1] RYOJI ASAHI, Toyota Central R&D Labs., Inc., O.Y. KONTSEVOI, Northwestern University, U. MIZUTANI, Toyota Phys.&Chem. Res. Inst., T. TAKEUCHI, Nagoya University, A.J. FREEMAN, Northwestern University — To elucidate the Hume-Rothery electron concentration rule, we determined the self-consistent electronic structures of the $Al_{108}Ru_{24}Cu_6Si_6$ and $Al_{108}Fe_{24}Cu_6Si_6$ 1/1-1/1-1/1 approximants containing 144 atoms in each Pm-3 cubic unit cell using the full-potential linearized augmented plane wave (FLAPW) method [1], now running on massively parallel computer platforms. A significant pseudogap was found around the Fermi level for both alloys in the calculated densities of states, which should contribute to stabilization of the system. The FLAPW wave functions provide a direct observation of the Brillouin zone resonance in the Fermi surface [2]: a Fourier analysis of the wave functions confirms the Hume-Rothery matching rule $2k_F = K$ where the reciprocal lattice vectors K consist of {543}, {550}, and {710} planes highly degenerate at the N point. Consequently, an effective electron concentration per atom (e/a) was evaluated to be 0.8 for both Ru and Fe in these structures making a sharp contrast with the previously assumed empirical value of -2.7 proposed by Raynor [3]. [1] Wimmer et al., Phys. Rev. B **24**, 864 (1981). [2] Asahi et al., Phys. Rev. B **72**, 125102 (2005). [3] Raynor, Prog. Metal Phys. **1**, 1 (1949).

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