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Nota di contenuto	Introduction -- Statistical Physics of Multicomponent Alloys -- Electronic Structure Ab Initio -- Atomic Short-Range Order and Phase Stability of the Refractory High-Entropy Alloys -- Multiphase Behaviour in the TiNbMoTaW and TiVNbMoTaW High-Entropy Alloys -- Phase Stability of the Cantor-Wu Medium- and High-Entropy Alloys -- A Cautionary Tale: Treatment of the Magnetic State in the Cantor-Wu Alloys -- Compositional Order and Subsequent Magnetostriction in Fe1Ga (Galfenol) -- Summary, Conclusions, and Outlook.
Sommario/riassunto	This book provides a comprehensive overview of a computationally efficient approach for modelling the phase behaviour of multicomponent alloys from first principles, describing both short- and

long-range atomic ordering tendencies. The study of multicomponent alloy systems, which combine three or more base elements in near-equal ratios, has garnered significant attention in materials science due to the potential for the creation of novel materials with superior properties for a variety of applications. High-entropy alloys, which contain four or more base elements, have emerged as a particularly fascinating subset of these systems, demonstrating extraordinary strength and fracture resistance, among other desirable properties. The book presents a novel modelling approach for studying the phase behaviour of these systems, which is based on a perturbative analysis of the internal energy of the disordered alloy as evaluated within the Korringa–Kohn–Rostoker (KKR) formulation of density functional theory (DFT), using the coherent potential approximation (CPA) to average over chemical disorder. Application of a Landau-type theory to an approximate form of the Gibbs free energy enables direct inference of chemical disorder/order transitions. In addition, the perturbative analysis facilitates extraction of atom-atom effective pair interactions for further atomistic simulations. The connection between the arrangement of atoms in a material and its magnetic properties is also studied. By outlining and applying the proposed modelling techniques to several systems of interest, this book serves as a valuable resource for materials scientists, physicists, and chemists alike, seeking to understand and develop new alloy systems with enhanced materials properties.