

Bunker and Stern Respond: The impressive calculation of Vvedensky and Pendry¹ (VP) and the comparison with experiment in their Comment give additional support to the conclusions in our Letter. Our apparently opposite interpretation from that of VP stems from a misunderstanding by VP of our Letter, and we welcome the opportunity to clarify the point. The misinterpretation of our Letter stems from an ambiguity in the definition of the edge region. Our definition is based on an experimental viewpoint which defines the edge as the rapidly rising absorption region which ends approximately at a constant level about which fine structure occurs. In Fig. 1(b) of VP the edge region of the experimental curve covers the energy region from about -1 to $+11$ eV. It is normally not feasible to separate atomic and solid-state effects in this region of rapid variation because the atomic contribution alone is not known experimentally except for the special case of the monatomic noble gases. Only beyond this region (in fact, beyond about 15 eV in this case) is it possible to separate the two contributions by the assumption that the atomic contribution is smoothly varying and the fine structure is the condensed-state contribution. It is clear by the comparison with experiment that the state of the art of the theory as given by the VP calculation is not reliable enough to make that separation; hence the need for a separation based on the experimental measurements.

The discrepancy between the experimental results and the full MS calculation is larger than the difference between the "full MS" calculation and the "type-1 MS only" features of the experimental curve past 5 eV, and we do not find any convincing objective criteria by which to decide whether one calculation is better than the other, particularly when one realizes

that the energy origin between the calculation and the measurement is a free parameter used in obtaining the best fit. This conclusion is only further strengthened when one includes only the region beyond our definition of the edge, namely beyond 11–15 eV.

The VP calculation confirms our theoretical argument that type-2 MS among the first-shell Ni atoms is negligible because they are octahedrally coordinated to the center atom. We note that the type-2 MS between the second-shell oxygens is a most favorable case because of the highly symmetric and large number of atoms which contribute 48 equivalent double-scattering terms to the largest contribution. In spite of this extremely favorable condition, the type-2 MS contribution is less than the type-1 MS throughout, verifying that the more physical perturbation expansion picture of XANES is an appropriate description. It should be noted that type-1 MS as defined in our Letter is not equivalent in all cases to intershell MS, as VP suggest. We are pleased that our intentionally aphoristic Letter has stimulated others to analyze the underlying physics, rather than just the behavior, of XANES.

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¹D. D. Vvedensky and J. B. Pendry, preceding Comment [Phys. Rev. Lett. **54**, 2725 (1985)].