# MATTERS ARISING

## Bragg intensities near structural phase transitions

IN a letter to *Nature* Åsbrink and Hong reported an increase of X-ray reflection intensity and profile widths at the low-to-high-$V_3O_5$ phase transition state[1]. The oldest reference I know of to the increase of X-ray intensity near structural phase transitions is that of De Quervain[2] in 1944. The effect was observed in a ferroelectric material (KDP) of which large rather perfect crystals can easily be grown. As these crystals show severe extinction, any disturbance caused by a phase transition is liable to increase the reflectivity. Since then, this effect has been observed rather often near first-order phase transitions, and also with neutron or γ-ray scattering[3]. It has been used as a very accurate indication for the occurrence of the transition[4,5] in a pressure cell. (We commonly use a series of crystals with various transition temperatures for accurate cryostat calibration.)

As this overshooting concerns integrated intensities, the width of the reflection profiles also increases. Various authors have used the information which lies in the variation near the transition of the profile shapes to characterise the state of the crystal near $T_c$. For example, Zeyen *et al.*[6,7] have studied the reflection profiles of DKDP crystals during its ferroelectric first-order phase transition using high precision cryogenics[8] and high resolution neutron diffraction techniques[9]. They investigated the spatial distribution of the phase mixing at $T_c$ where both the paraelectric and the ferroelectric phases coexist in the crystal in a particular arrangement which actually minimises elastic and electrostatic (polarised domains) energies and depends on the structural change at $T_c$. Following their model the DKDP crystal forms a multilayer of alternating paraelectric and ferroelectric sheets. It explains directly the overshooting intensity near $T_c$. The existence of these layers has in the meantime been confirmed directly by optical observation in a special cryostat[10]. Other systems giving different spatial arrangements have also been studied.

C. M. E. ZEYEN
*Institut Laue-Langevin,*
*156X,*
*38042 Grenoble Cedex, France*

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ÅSBRINK AND HONG REPLY—We thank Zeyen for information on early discussions about intensity overshoot in connection with studies on $KH_2PO_4$ and $KD_2PO_4$.

The possibility of phase mixing during the transition occurred to us; however, we had to discard it as several reflections did not even exhibit the profile widening at $t_T = 154.7$ °C required by the difference in unit cell dimensions between the two $V_3O_5$ phases. (We made the comparative profile width measurements at 153 and 156 °C for low- and high-$V_3O_5$, respectively, and assumed that the entire change of unit cell dimensions between those temperatures took place at $t_T$.)

STIG ÅSBRINK
SAM-HYO HONG
*Department of Inorganic Chemistry,*
*Arrhenius Laboratory,*
*University of Stockholm,*
*Fack, S-106 91 Stockholm, Sweden*

## Magnetostratigraphy, biostratigraphy and geochronology of Cretaceous–Tertiary boundary sediments, Red Deer Valley

LERBEKMO *ET AL.*[1] have presented some valuable radiometric data from an important continental sedimentary sequence which includes the Cretaceous–Tertiary boundary in Alberta. However, the palaeomagnetic data which they presented in their Fig. 2 show considerable scatter and do not provide a well defined polarity zonation.

Lerbekmo *et al.* correlate their magnetic polarity zonation from the Red Deer Valley with the magnetic polarity time scale. They note that the Cretaceous–Tertiary boundary, as recognised by marine biozonations, occurs near the base of anomaly 29. Lerbekmo *et al.* then concluded that the long normal polarity zone overlying the Cretaceous–Tertiary boundary in the Red Deer Valley, as recognised by dinosaur extinction and palynofloral zones, must correlate with anomaly 29. We consider this correlation to be circular reasoning based on the incorrect presumption that the Cretaceous–Tertiary boundary in the Red Deer Valley is synchronous with the Cretaceous–Tertiary boundary as determined by marine biozonations. This normal polarity zone in the Red Deer Valley could correlate with anomaly 28 or even anomaly 27. The magnetic polarity zonation in the Red Deer Valley does not show a convincing correlation to the magnetic polarity time scale. Thus, the conclusions reached by Lerbekmo *et al.* based on their correlation are rather speculative.

In addition, Lerbekmo *et al.* proposed an alternative to our[2,3] correlation between the San Juan Basin magnetic polarity zonation and the magnetic polarity time scale. They suggested that the normal polarity zone which we correlated with anomaly 29 should be correlated with a normal polarity interval between anomalies 29 and 30. However, there is no evidence for such a normal polarity interval in either of the two magnetostratigraphic sections at Gubbio, Italy[4,5] nor in the magnetostratigraphic section at Moria, Italy[6] nor in the marine magnetic anomaly record[7]. The palaeomagnetic data from the San Juan Basin provide a well defined magnetic polarity zonation which shows a strong correlation with the magnetic polarity time scale[2,3]. We do not agree with Lerbekmo *et al.*'s reinterpretation of our data.

Lastly, we do not agree that there are "palaeontological discrepancies between the New Mexico, Alberta, and Gubbio, Italy sections with respect to the Cretaceous–Tertiary boundary". As we pointed out[2], the Cretaceous–Tertiary boundary is defined by extinction of marine invertebrates but is recognised in terrestrial sedimentary sequences by the last occurrence of dinosaur fossils. These two biological events need not have occurred synchronously and marine/non-marine intertonguing relationships do not provide enough precision to test for global synchroneity of this geological-time boundary. However, magnetostratigraphy does provide a possible technique for determining the temporal relationship of dinosaur extinction and marine invertebrate extinctions marking the Cretaceous–Tertiary boundary. Thus our magnetostratigraphic data which indicate a lack of synchroneity between dinosaur extinction in the San Juan Basin and the Cretaceous–Tertiary boundary at Gubbio, Italy do not constitute a palaeontological discrepancy as implied by Lerbekmo *et al.*

ROBERT F. BUTLER
EVERETT H. LINDSAY
*Department of Geosciences,*
*University of Arizona,*
*Tucson, Arizona 85721*

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