Figure 2
Upper panel displays unpolarized experimental S K edge spectrum of TiS$_2$ (chain line) as taken from Wu et al (1996) together with polarized projected DOS calculated by pseudopotential method and broadened by two different lorentzians. Lower panel shows polarized Te L_1 edge spectrum of TiTe$_2$, both experimental and calculated using the RS-MS method. As in Fig. 1, solid lines represent polarized components parallel to Ti layers, dashed lines stand for components perpendicular to Ti layers.

ambiguous: While the polarization dependence of the peaks seems to be similar in both compounds, there is a clear difference between the broad double peak around 4950 eV in TiTe$_2$ and the unique peak at 2476 eV in TiS$_2$.

The influence of the size of the cluster on Ti spectrum of TiS$_2$ is investigated in Fig. 3. Our results support the conclusion of Wu et al (1997) that the anisotropic pre-peak is generated by Ti atoms in the second coordination shell. Most significant features of the spectrum are converged if 51 atoms (eight coordination spheres) are included.
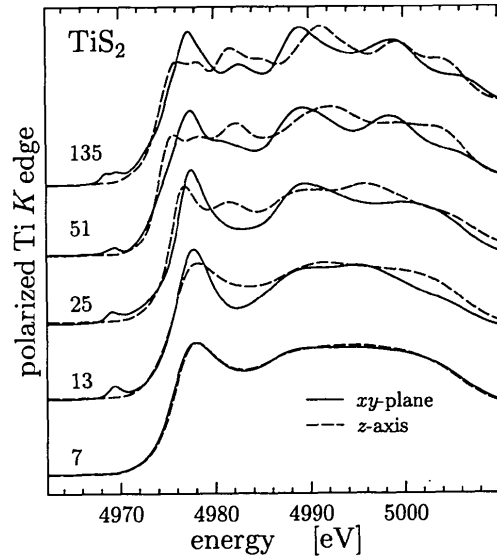
Figure 3
Polarized Ti K edge spectra of TiS$_2$ calculated for varying cluster sizes. The number at each curve indicates number of atoms contained in the corresponding cluster.

3. Results and discussion

In Fig. 1, theoretical and experimental Ti K edge polarized spectra of TiS$_2$, TiSe$_2$, and TiTe$_2$ in equivalent energy scales are presented. There is an apparent correlation between spectral features of the three compounds. The selfconsistent pseudopotential calculation confirms the suitability of non selfconsistent Mattheiss potential for this study. The largest discrepancy between the theoretical and experimental curves occurs in the region above the main peak for all three compounds (4980-4985 eV). The disagreement is most prominent in TiS$_2$ (see also unpolarized study of Wu et al 1997), while the TiSe$_2$ experimental spectrum is described remarkably better in this region by the theory. Hence we tentatively ascribe this disagreement to multielectron effects — the simple phenomenological linearly energy-dependent Lorentzian broadening probably is not good enough to describe inelastic losses in TiS$_2$ properly.

A complementary study of Te L_1 spectrum of TiTe$_2$ and S K spectrum of TiS$_2$ is shown in Fig. 2 (again in equivalent energy scales). The TiTe$_2$ spectrum contains the low-energy tail (pre-peak) of the Ti K edge, too. For TiS$_2$, unpolarized experiment of Wu et al (1996) is displayed together with polarized density of states (DOS) broadened to account both for the $1s$ core hole lifetime in S (0.59 eV) and for the $2s$ core hole lifetime in Te (3.32 eV). The correspondence between features of TiTe$_2$ and TiS$_2$ spectra is a bit

Figure 4
Polarized Te L_1 edge spectra of TiTe$_2$ calculated for varying cluster sizes. The number at each curve indicates number of atoms contained in the corresponding cluster.

The cluster size convergence of Ti spectra of $TiSe_2$ and $TiTe_2$ exhibits the same pattern as in the case of TiS_2, so we do not display corresponding sets of curves here for brevity.

In Fig. 4, cluster size effect for the Te spectrum of $TiTe_2$ is examined. The convergence with cluster size is slower than in the case of Ti edge in TiS_2 (or, equivalently, in $TiTe_2$): Three coordination spheres are needed to reproduce the first peak correctly (at 4941 eV) and even as much as 57 atoms are not enough to describe the double structure of the second peak around 4950 eV (well-resolved in experiment — cf. Fig. 2).

This is similar to the cluster size convergence of K spectra of ZnS, which is essentially quicker for the Zn edge than for the S edge (Sainctavit *et al* 1987). The explanation proposed by Sainctavit *et al* utilizes the fact that the scattering cross section of Zn (as well as Ti) atoms is roughly smaller by half than the cross section of chalcogen atoms in the relevant energy region. Hence it was suggested that the key factor influencing the cluster size convergence is the number of *chalcogen atoms* contained in the cluster rather then the total number of atoms. A more detailed study would be needed to elaborate this conjecture for transition metal dichalcogenides.

References

Bocharov, S., Dräger, G., Heumann, D., Šimůnek, A. & Šipr, O. (1998). *Phys. Rev.* **B58**, 7668–7674.

Bödicker, A. & Schattke, W. (1997). *Phys. Rev.* **B55**, 5045–5050.

Claessen, R., Anderson, R. O., Gweon, G.-H., Allen, J. W., Ellis, W. P., Janowitz, C., Olson, C. G., Shen, Z. X., Eyert, V., Skibowski, M., Friemelt, K., Bucher, E. & Hüfner, S. (1996). *Phys. Rev.* **B54**, 2453–2465.

Dräger, G., Frahm, R., Materlik, G. & Brümmer, O. (1988). *phys. stat. sol.* (b) **146**, 287–294.

Fang, C. M., de Groot, R. A. & Haas C. (1997). *Phys. Rev.* **B56**, 4455–4463.

Heumann, D., Hofmann, D. & Dräger, G. (1995). *Physica* B **208&299**, 305–306.

Sainctavit, P., Petiau, J., Calais, G., Benfatto, M. & Natoli, C. R. (1987). *J. Phys. (Paris)* **48**, C9-1109–C9-1112.

Šimůnek, A., Šipr, O., Bocharov, S., Heumann, D. & Dräger, G. (1998) *Phys. Rev.* **B56**, 12232–12237.

Vackář, J., Hytha, M. & Šimůnek, A. (1998). *Phys. Rev.* **B58**, *to be published.*

Vvedensky, D. D., Saldin, D. K. & Pendry, J. B. (1986). *Comput. Phys. Commun.* **40**, 421–440.

Wu, Z. Y., Lemoigno, F., Gressier, P., Ouvrard, G., Moreau, P., Rouxel, J. & Natoli, C. R. (1996). *Phys. Rev.* **B54**, 11009–11013.

Wu, Z. Y., Ouvrard, G., Moreau, P. & Natoli, C. R. (1997). *Phys. Rev.* **B55**, 9508–9513.