doi: 10.1017/S1431927609095488
Microsc Microanal 15(Suppl 2), 2009

Background Removal Methods Applied to Atom Probe Data

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Quantitative information can be extracted from atom probe mass spectra using the same general techniques used in other spectroscopic methods [1]. A major challenge is to accurately quantify minor components in a high-background environment. We evaluate how well this challenge is met by measuring the isotopic abundance of Ni^{++} isotopes in a steel sample collected using the local electrode atom probe (LEAP®)3000 XHR microscope[2.3].

The time-of-flight (TOF)-independent background can be estimated easily and removed from the spectrum. While this is of itself useful in some cases, it produces poor results presented here due to the relatively long tails from the lower mass peaks that dominate the Ni background. Fig. 1 shows how the TOF-independent background underestimates the true background for ions with mass-to-charge-state ratios greater than 25 Da. The measured isotopic abundance using this simple background estimate is shown in Table 1 under the "TOF-independent" column. The abundances for this and all results presented here were computed using the ranges shown after decomposition of the Fe/Ni peak overlap at 29 (about 92.6% of which is Ni)

A simple yet robust TOF-dependent background correction method consists of averaging the spectrum just below each mass window and subtracting this pre-peak sideband average. Fig. 2 shows a detail of the spectrum containing the Ni^{++} peaks. The areas under these background lines (red rectangular shapes) were subtracted from the windowed counts (shaded ranges) and the results are shown in Table 1 under the "Sideband sampled" heading. The sum of the squared error-weighted deviations of the measurements from the natural abundance (i.e. χ^2) is 16, reasonable agreement for four degrees of freedom

Another method of estimating the TOF-dependent background relies on specific knowledge about the peak shape. Fig. 3 shows thermal tails sometimes encountered in laser APT data [2]. The red curve is a fit to the tail of the $^{52}Cr^{++}$ peak made just below the $^{53}Cr^{++}$ peak and extrapolated to higher masses. This represents the background contribution from the $^{52}Cr^{++}$ peak to all higher masses. A peak-stripping method was employed, where the procedure of fitting and subtracting was repeatedly applied to the spectrum starting at the lowest mass peak and continuing to higher values in the spectrum. Fig. 4 shows the Ni^{++} region after the stripping has been applied. There is still some residual shape to the region between peaks and this was accounted for using the sideband method described above. The results of this calculation are in Table 1 under the Peak stripping heading. These measurements are in very good agreement with a χ^2=2.3 for four degrees of freedom.

In situations where the signal-to-background ratio is small (< 1 in the case of $^{64}Ni^{++}$) it is important to accurately estimate the background level. Two methods of estimating the TOF-dependent background are presented here. While the peak-stripping method gives the best result, the sideband method results are also very good and do not depend on any model assumptions.

[1] R. Egerton, Ultramicroscopy 3 (1978) 243.
[2] J. H. Bunton et al., Microsc. Microanal. 13 (2007) 418.
[3] P. H. Clifton et al., Microsc. Microanal. 14(S2) (2008) 454.

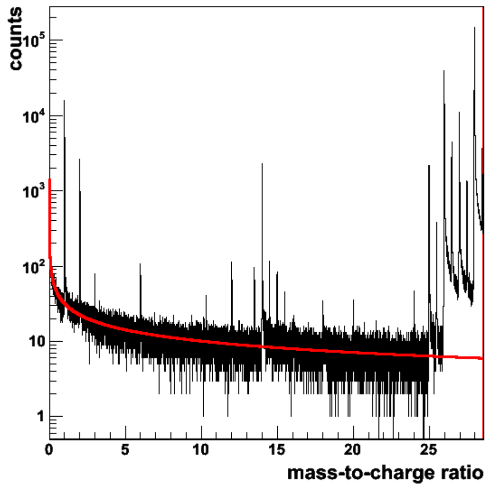

Fig. 1 TOF-independent background fit superimposed spectrum showing inaccurate fitting above ~25 Da.

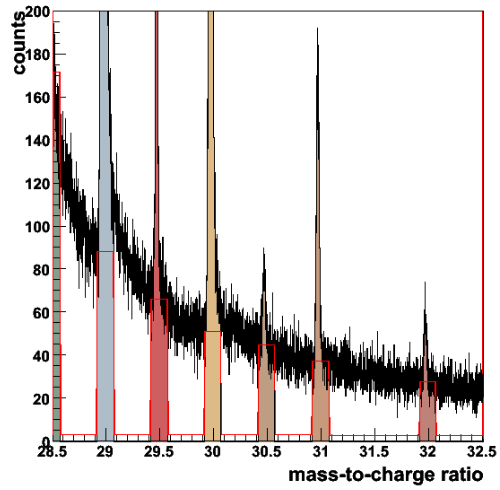

Fig. 2 Spectrum detail showing sideband-sampled background level within shaded ranges and TOF-independent background level between shaded ranges.

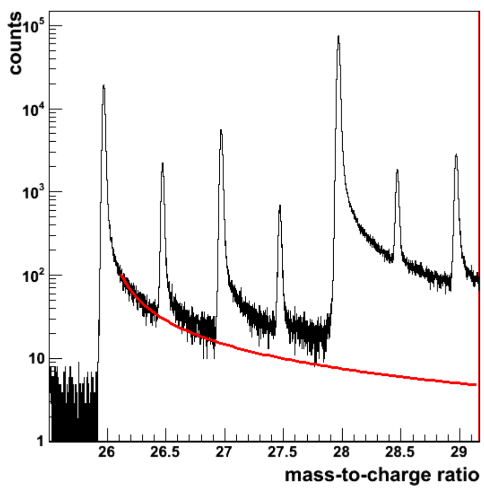

Fig. 3. Thermal model fit to $^{52}Cr^{++}$ tail.

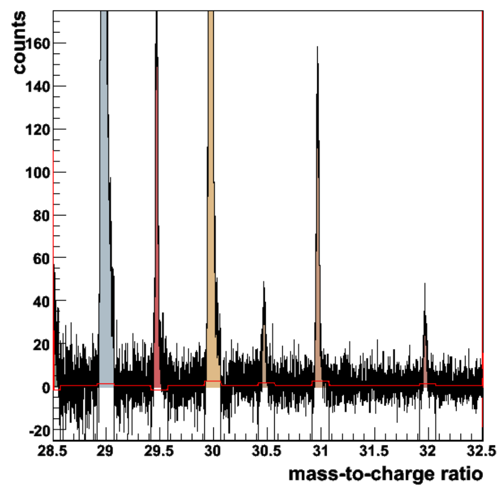

Fig 4. Same as Fig. 2, but after peak stripping.

TABLE 1. Comparison of Ni^{++} isotopic abundance measurements (only statistical errors shown), SD = number of standard deviations.

Ni Isotopes	Natural Abundance	TOF Independent		Sideband Sampled		Peak Stripping	
		Measured	SD	Measured	SD	Measured	SD
58	68.27%	61.26±0.12%	58	68.36±0.15	0.6	68.12±0.13	1.2
60	26.10	24.84±0.11	11	26.33±0.14	1.6	26.16±0.14	0.4
62	1.13	4.75±0.06	60	0.90±0.07	3.3	1.16±0.07	0.4
63	3.59	6.08±0.06	41	3.56±0.08	0.4	3.65±0.08	0.8
64	0.91	3.07±0.05	43	0.85±0.06	1.0	0.91±0.06	0.0
χ^2			1e4		16		2.3

https://doi.org/10.1017/S1431927609095488 Published online by Cambridge University Press