

## CHAPTER 8 CONCLUSIONS & FUTURE WORK

This thesis has reached the following conclusions:

- 1) *Under most irradiation conditions, chromium enriches at grain boundaries in F-M alloys, and this observation can be explained by differences in solute-defect diffusion rates.* Consistent Cr enrichment has been observed in all four alloys studied in this work--T91, HCM12A, HT9, and a 9Cr model alloy—over a wide temperature range of 300-600°C, at doses of up to 10 dpa. Only one instance of Cr depletion has been observed, in T91 irradiated to 3 dpa at 700°C. Chromium RIS in F-M alloys occurs in small amounts; no more than 2.5 wt% Cr enrichment was ever recorded. These behaviors are in quite stark contrast to Cr RIS tendencies in austenitic steels, in which Cr depletion of up to 20 wt% has been routinely measured.

The inverse Kirkendall mechanism can explain the observed differences in Cr RIS between F-M and austenitic alloys. In austenitic alloys, the diffusion coefficient ratio of Cr to Ni for vacancies is greater than unity, while that for interstitials is less than unity, particularly in the temperature range of interest. The relative magnitude of these ratios mean that RIS in austenitic steels should be dominated by Cr transport via vacancies, resulting in Cr depletion. In addition, because the difference between the vacancy and interstitial diffusion coefficients is rather large, the expected amount of RIS will also be large.

However, in F-M alloys, the diffusion coefficient ratios of Cr to Fe for vacancies and for interstitials are both greater than unity and are of almost identical magnitudes. This means that both vacancies and interstitials are causing Cr RIS, the vacancies causing depletion and the interstitials, enrichment. At any particular temperature, whichever diffusion coefficient ratio—that for vacancies, or that for interstitials—is greater will decide the direction of RIS. In most of the conditions studied in this thesis, the interstitial

diffusion coefficient was greater than that for vacancies, causing the observed Cr enrichment. And since the vacancy and interstitial diffusion coefficients are similar in magnitude, the difference between them is small, so the expected amount of RIS will also be small.

2) *A “crossover” from Cr enrichment to Cr depletion occurs between 600°C and 700°C in alloy T91, and this provides further confirmation for the inverse Kirkendall mechanism of Cr RIS in F-M alloys.* In alloy T91 irradiated to 3 dpa, Cr enrichment is observed at 600°C, and Cr depletion at 700°C. The temperature interval in which the crossover occurs is consistent with the crossover predicted by the diffusion coefficient ratios of Cr to Fe for vacancies and for interstitials. As mentioned in the preceding paragraph, the diffusion coefficient ratios in F-M alloys are similar in magnitude. But small differences in their slopes cause the vacancy and interstitial diffusion coefficient ratios to cross one another near ~660°C. At temperatures below the crossover temperature, the diffusion coefficient ratio for interstitials exceeds that for vacancies, which can explain the observed Cr enrichment in T91 irradiated between 300°C and 600°C. But above the crossover temperature, the diffusion coefficient ratio for vacancies becomes greater than that for interstitials, which explains the observed Cr depletion in T91 at 700°C. The existence of a crossover behavior is particular to the F-M alloy system. The existence of a crossover between Cr enrichment and Cr depletion in F-M alloys provides support for the inverse Kirkenall mechanism.

3) *The amount of Cr enrichment decreases with increasing bulk Cr concentration, and this behavior can also be attributed to differences in diffusion rates between atomic species.* Chromium enrichment is measured in T91, HCM12A, HT9, and the 9Cr model alloy following 3 dpa irradiation at 400°C. The amount of Cr enrichment is observed to decrease as a function of increasing bulk Cr concentration. The inverse Kirkendall model calculates a consistent behavior, as long as Cr-composition-dependent interstitial migration energies for both Fe and Cr are input into the model. Composition-dependent interstitial migration energies are calculated for bulk Cr concentrations less than or greater than 9 wt% Cr; the migration energies for 9 wt% Cr are fixed at their original values.

The decreasing amount of Cr with increasing bulk Cr concentration, as measured in the 400°C experiment, can be explained by differences in atomic diffusion rates.

When composition-dependent interstitial migration energies are used for alloys with bulk Cr concentration > 9 wt%, the diffusion coefficient ratio of Cr to Fe for interstitials decreases slightly in magnitude, causing two major effects. First, the predicted crossover temperature decreases, although Cr is still calculated to enrich at the experiment temperature of 400°C. Second, the Cr-to-Fe interstitial diffusion coefficient ratio moves closer to that of vacancies at 400°C. The difference between the two diffusion coefficient ratio lines becomes even smaller, and thus, the expected amount of Cr RIS should be even smaller than at lower bulk Cr concentrations.

4) *The experimentally observed Cr RIS behaviors cannot be attributed to the solute drag mechanism.* When the solute drag mechanism is incorporated into the IK model using a positive Cr-interstitial binding energy, unreasonably large amounts of Cr enrichment are calculated. Conversely, when the solute drag mechanism implements a positive Cr-vacancy binding energy, unreasonable quantities of Cr depletion are calculated. Clearly, the solute drag mechanism results in Cr RIS that is entirely inconsistent with experimental measurements

6) *The behavior of Cr RIS—and thus, of Fe RIS, as well—in F-M alloys is largely consistent with the inverse Kirkendall mechanism and not consistent with the solute drag mechanism, supporting IK as the mechanism controlling Cr RIS in commercial F-M alloys.*

7) *Minor elements such as Si, Ni, and Cu, segregate by a different, yet undetermined mechanism, than that by which Cr and Fe segregate.* RIS of minor elements exhibit a different temperature dependence than does RIS of Cr and Fe. The temperature range over which the minor elements segregate is more limited (400-500°C) than that over which Cr and Fe segregate (at least 300-700°C). However, the driving mechanism of minor element RIS has not been determined.

While some notable conclusions have been reached in this work, there remain some unanswered questions that deserve future attention:

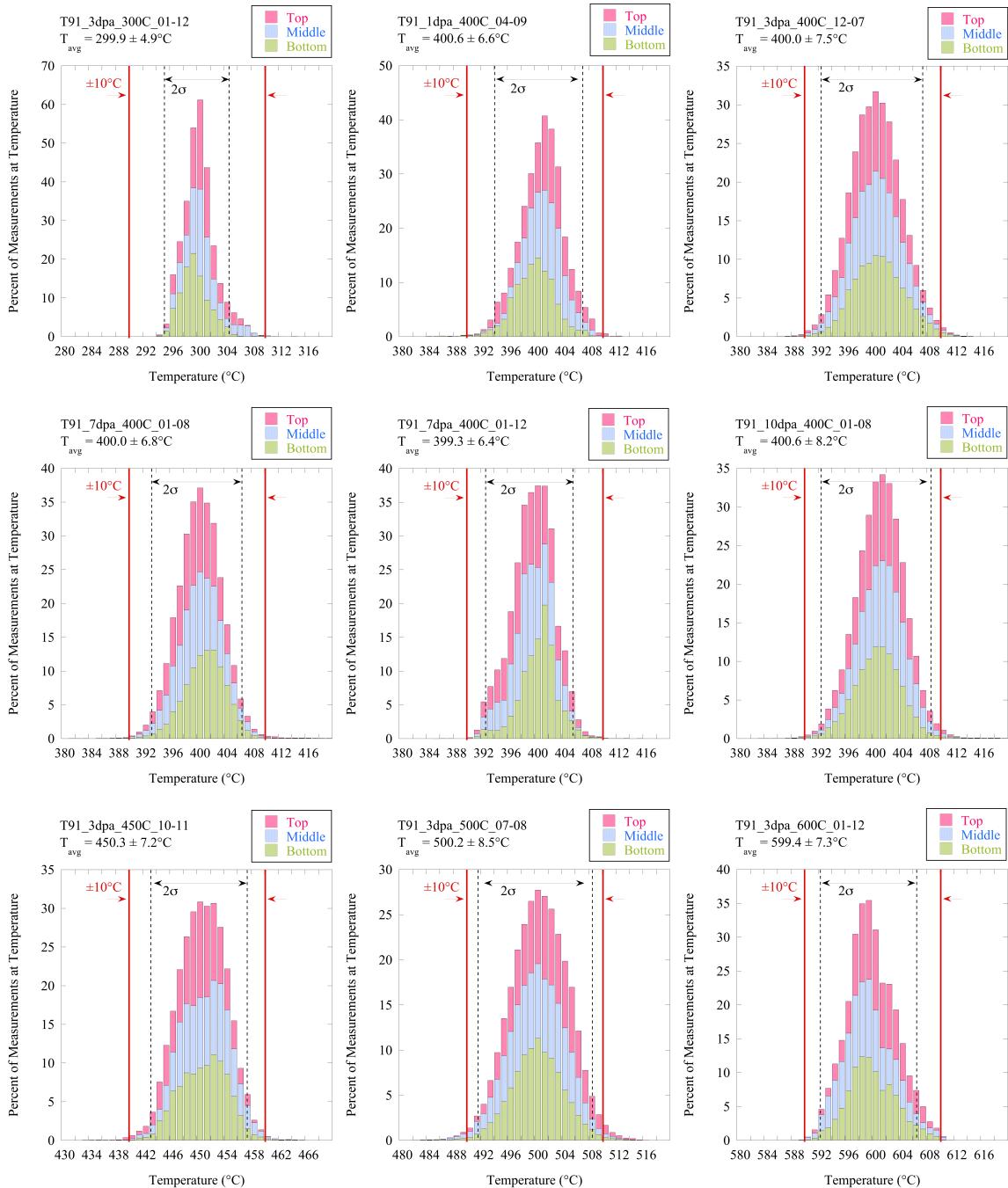
1) *There remain unresolved issues with the dose dependence of Cr RIS, especially with respect to the interrelationship of RIS and microstructure.* There are

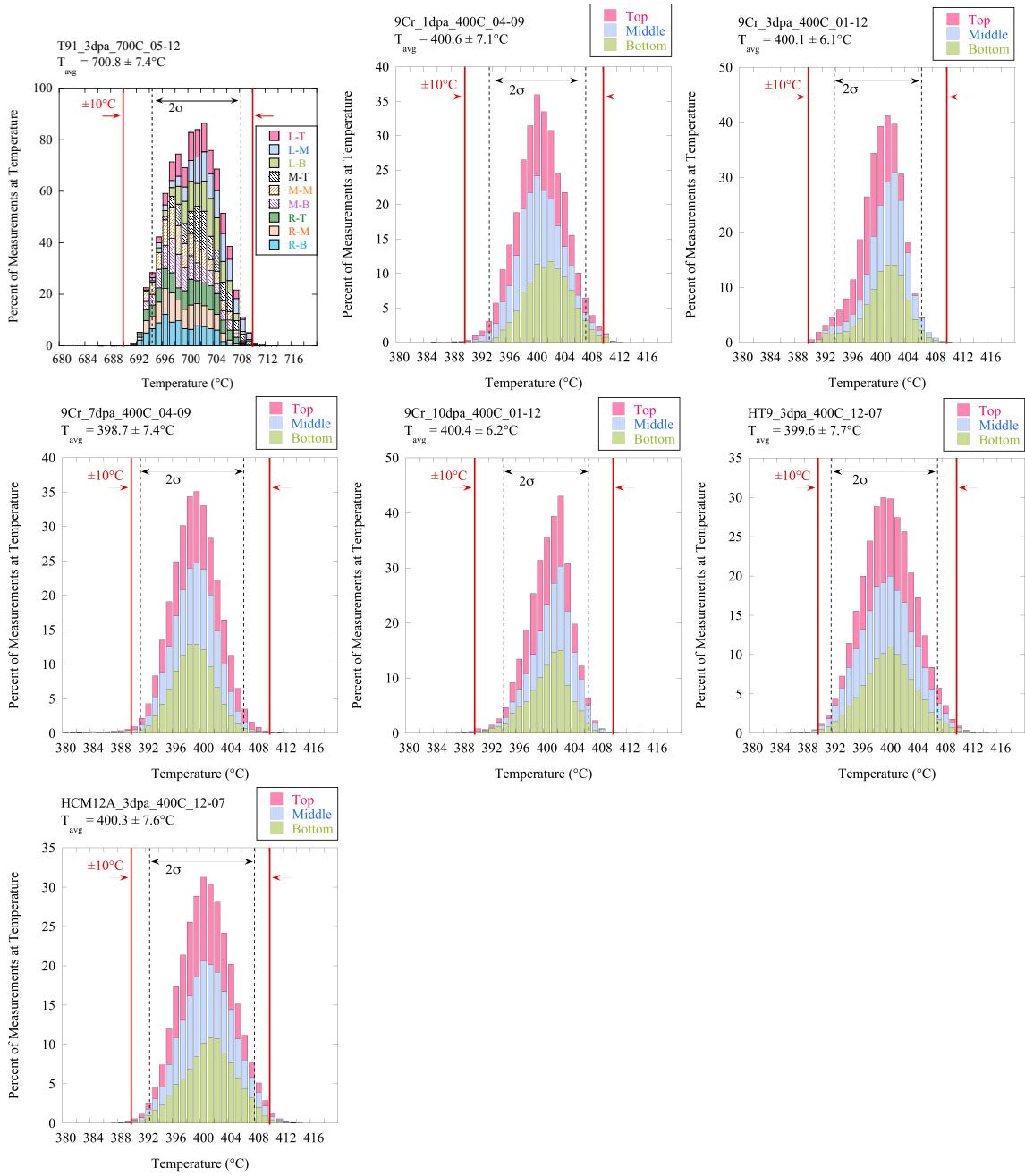
significant differences in the kinetics of RIS between the IK model and experiment, particularly regarding the onset of RIS and the onset of steady-state RIS. It is theorized that the model-experiment difference in the onset dose may be due to a microstructurally-related incubation period in the experimental steels. It is also theorized that the model-experiment difference in the steady-state RIS behavior is due to microstructural evolution. Future work could more closely study the microstructural issues and kinetics of RIS in the IK mechanism. In addition, studying RIS at the boundaries of microstructural features such as dislocation loops and precipitates, may offer further insight into the RIS-microstructure relationship.

2) *The RIS mechanism of minor elements in F-M alloys has yet to be determined.*

Work in this thesis, particularly in the modeling effort, has focused largely on Cr and Fe RIS. However, it has been concluded that minor elements Si, Ni, and Cu segregate by a different mechanism than that by which Cr and Fe segregate. This conclusion necessitates further study into the mechanism driving RIS of the minor elements. Furthermore, only a limited number of minor elements have been studied in this thesis, due to detectability issues with the STEM technique. Future work should use a technique capable of detecting a greater number of the constituent elements, in order to determine whether additional elements are segregating.

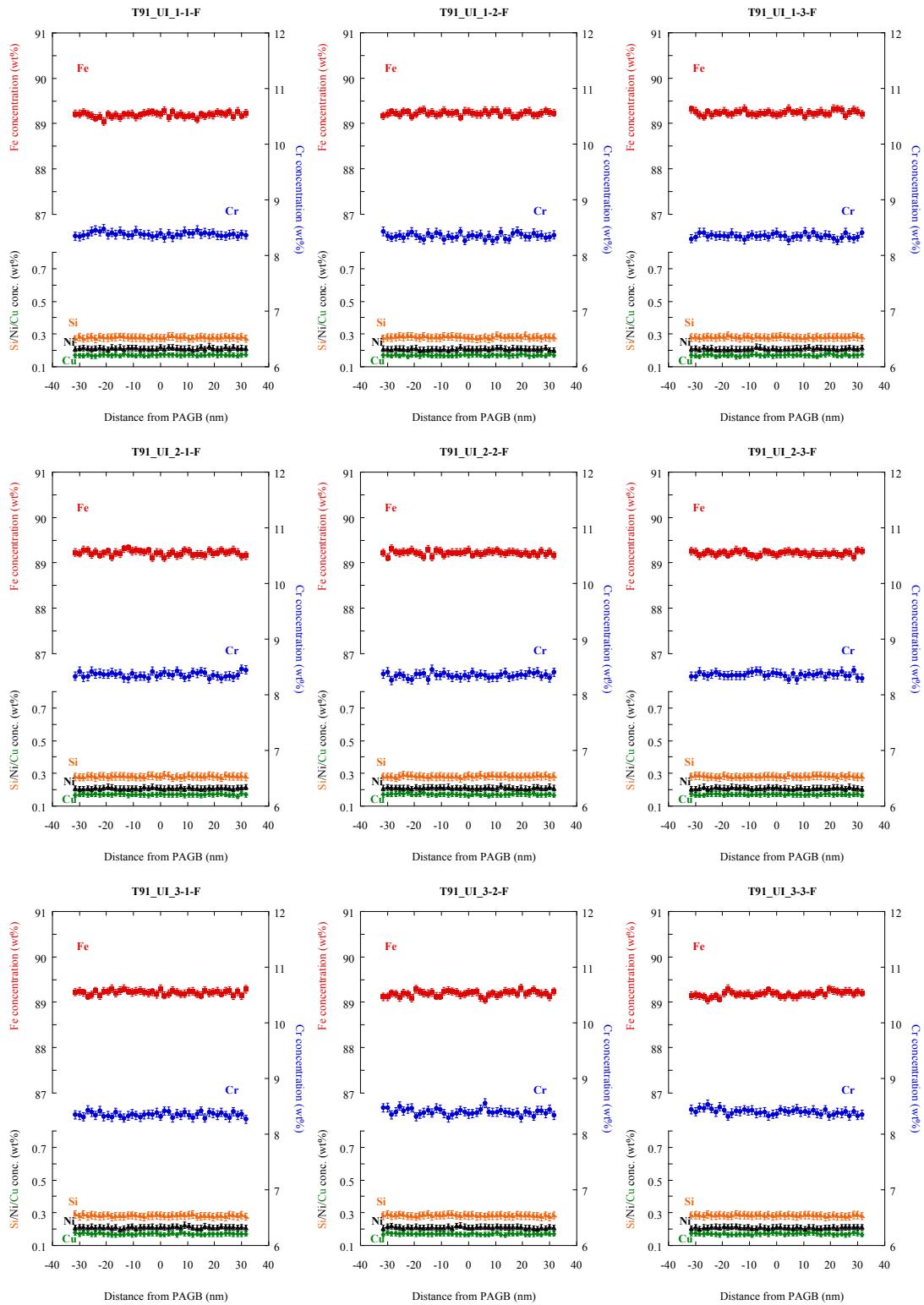
## **APPENDIX A: Temperature Histograms**

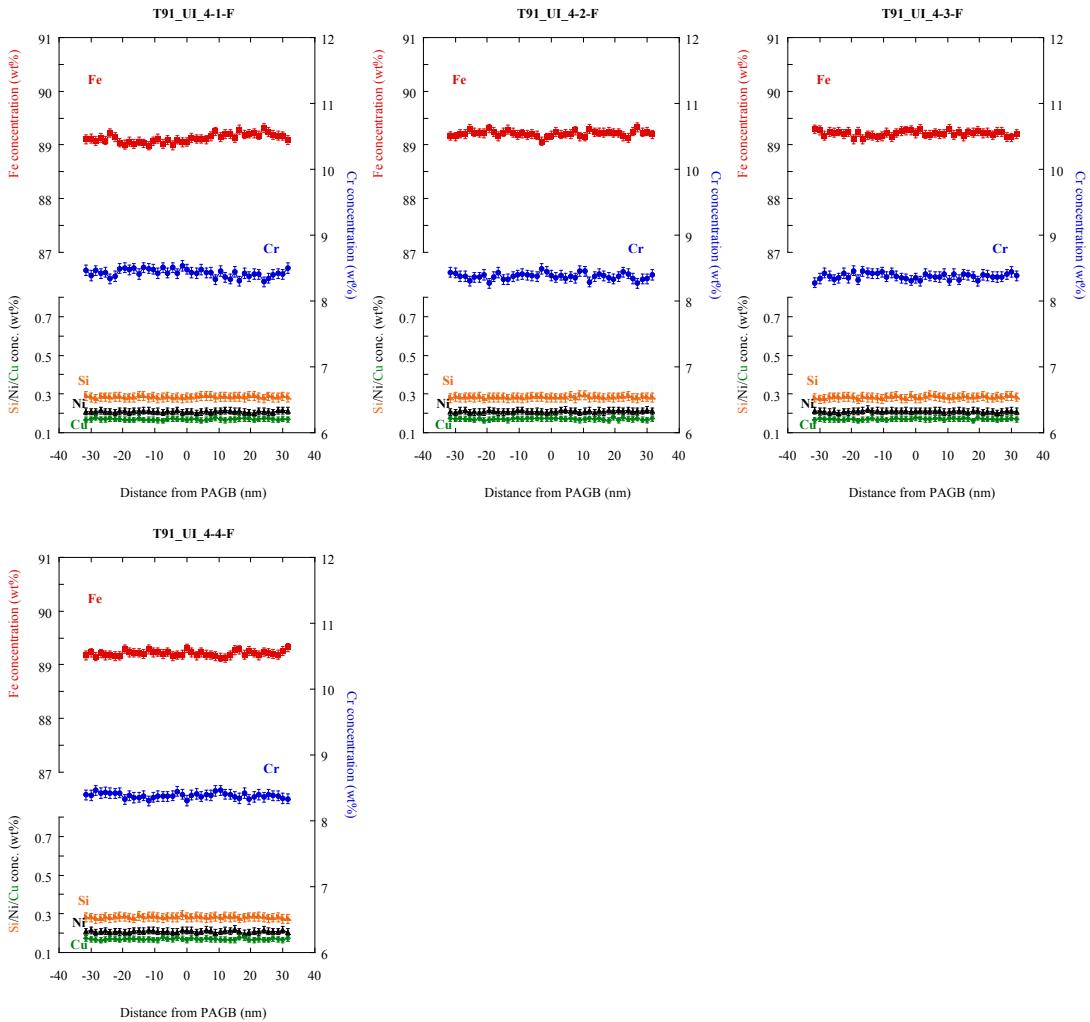




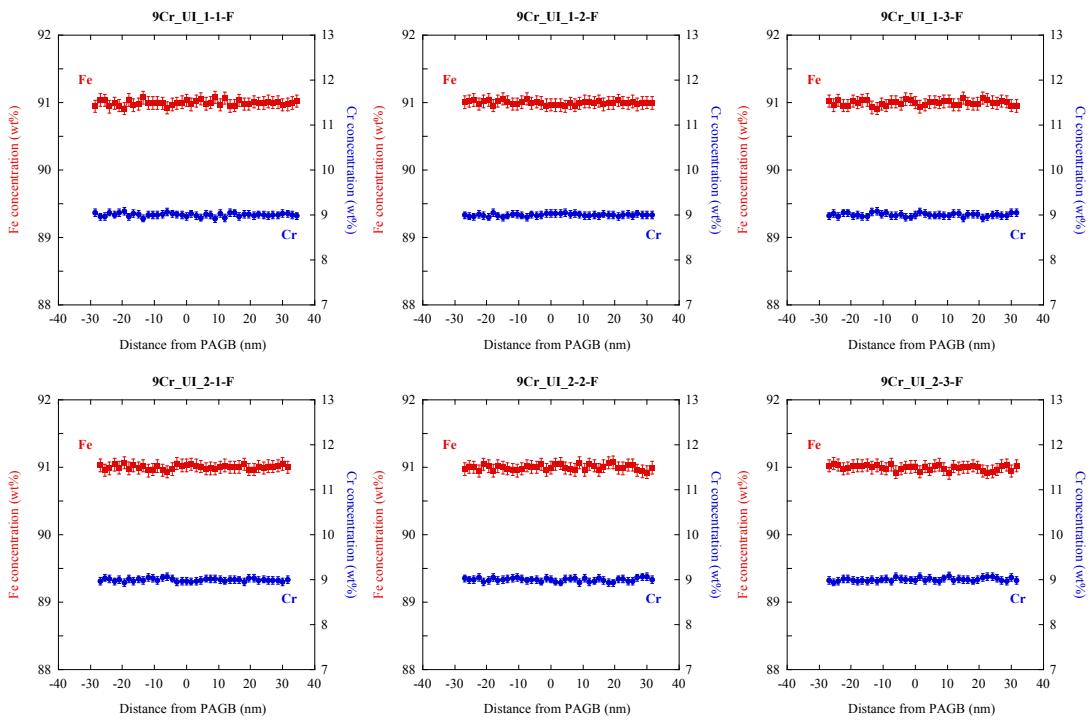
## **APPENDIX B: Composition Profiles**

## T91 UI

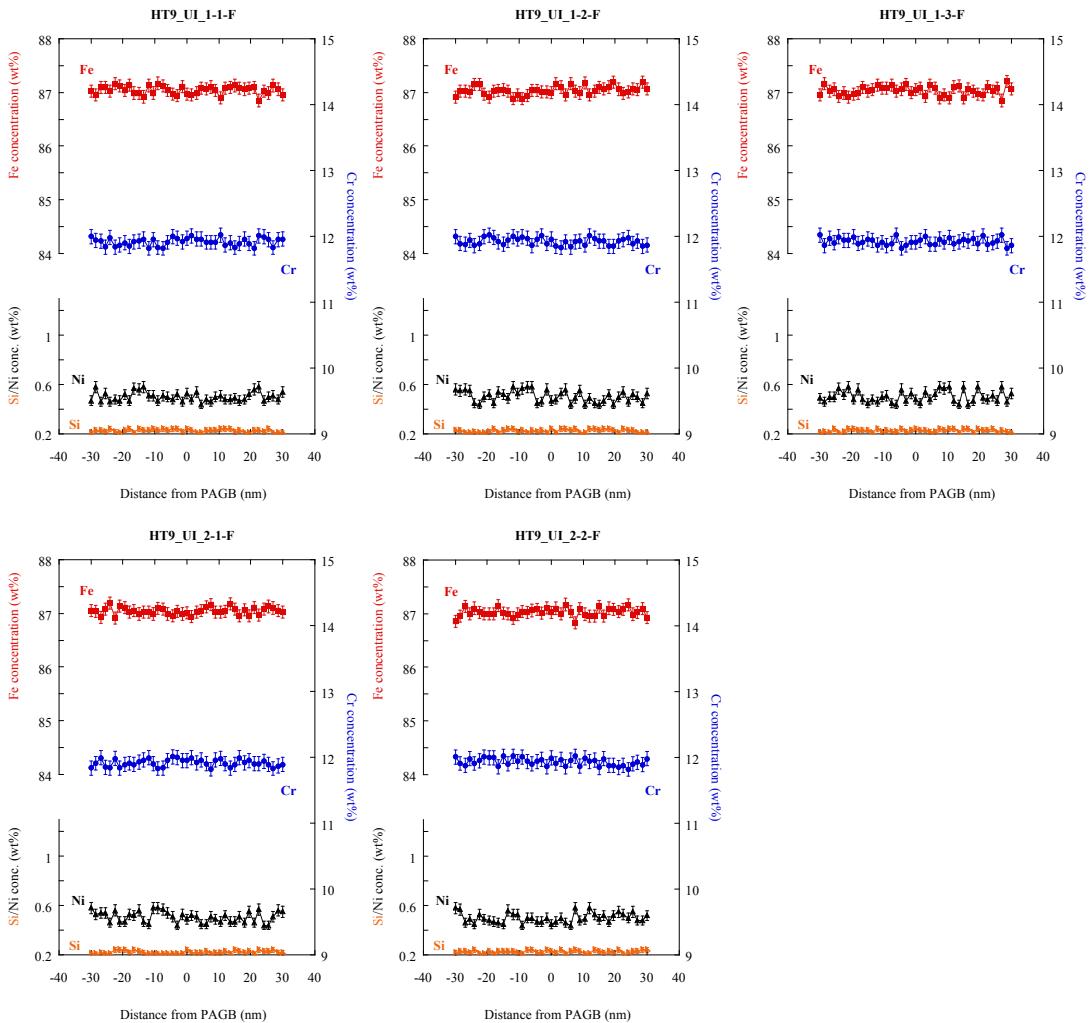




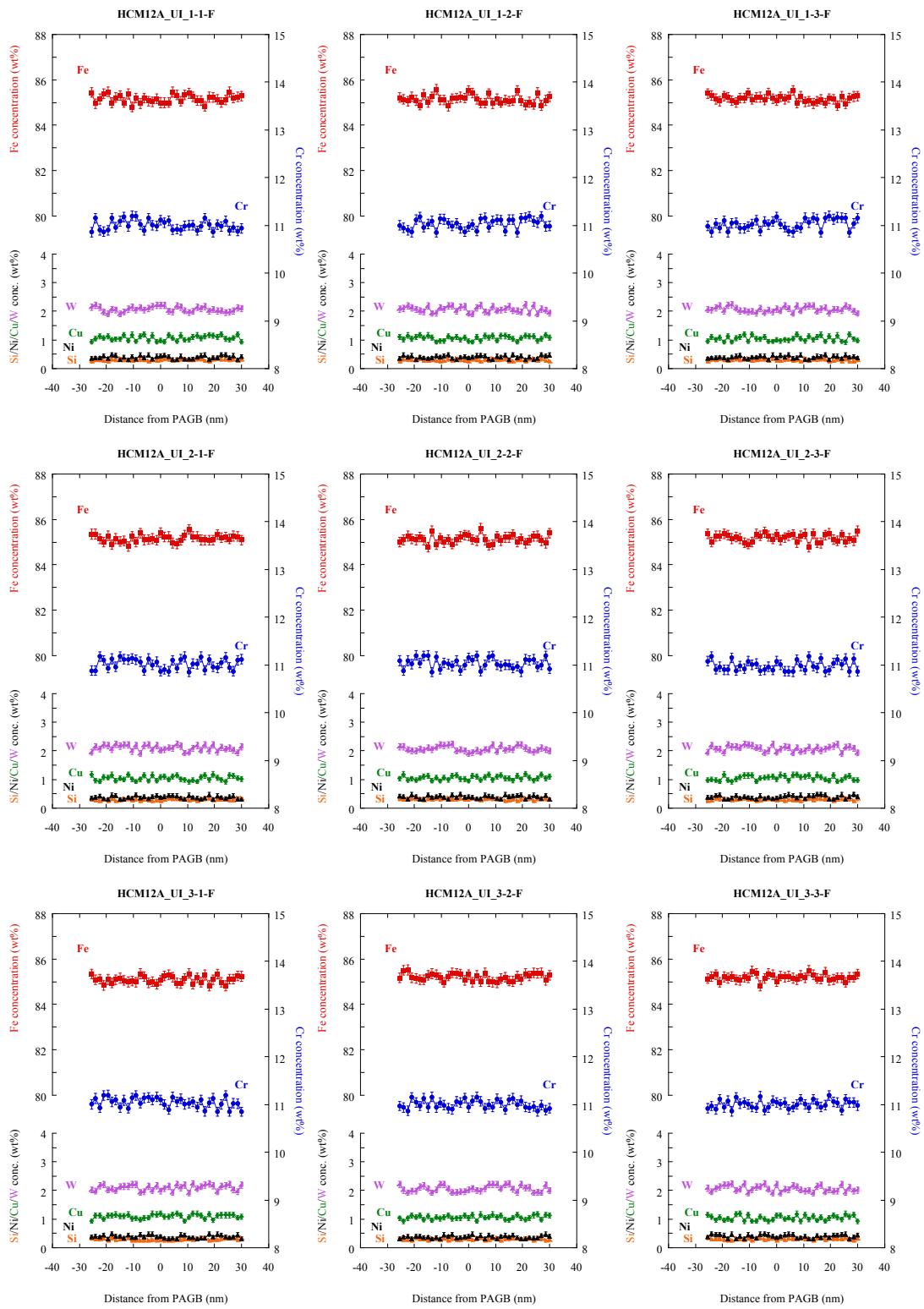
## 9Cr\_UI



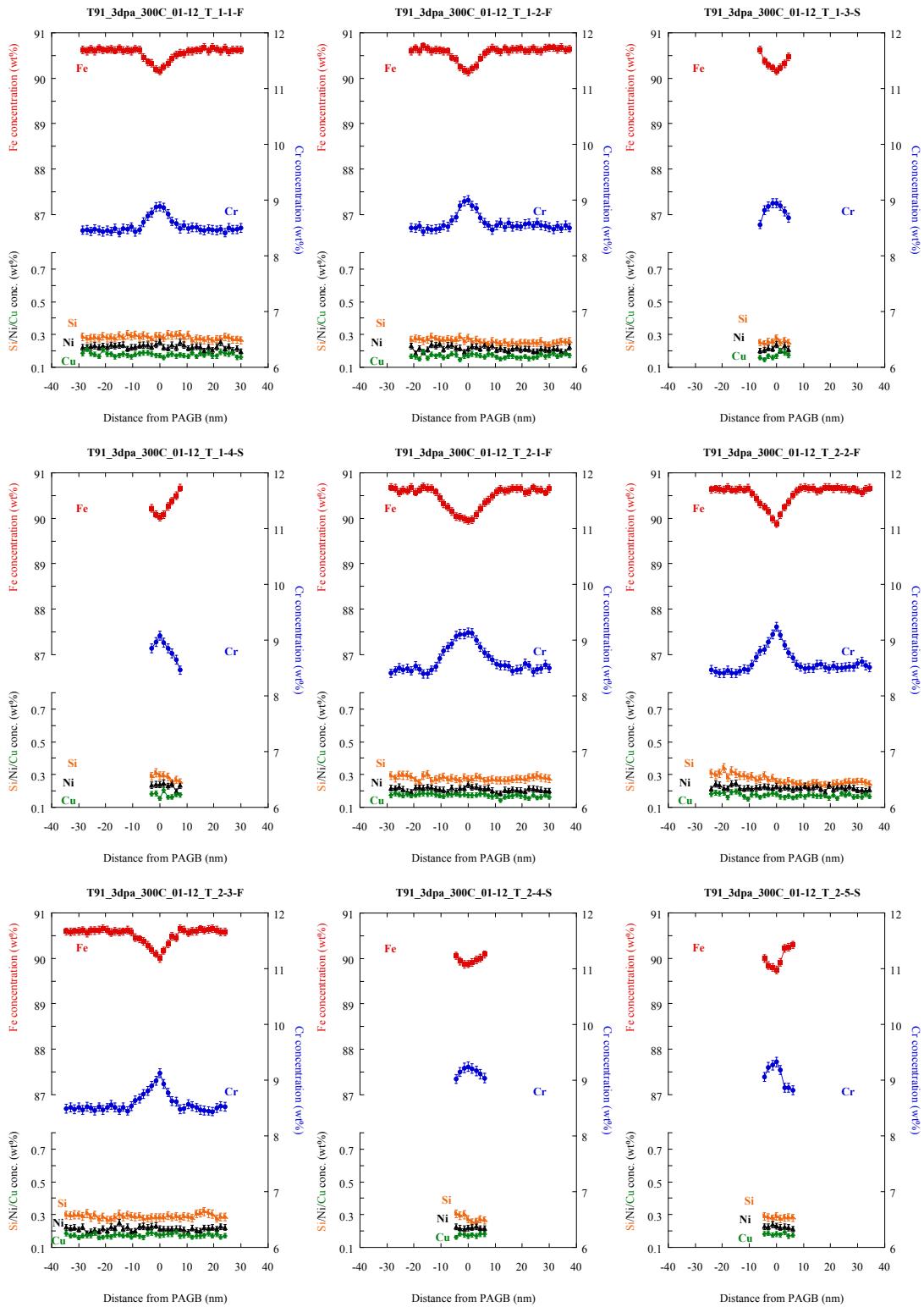
## HT9\_U1



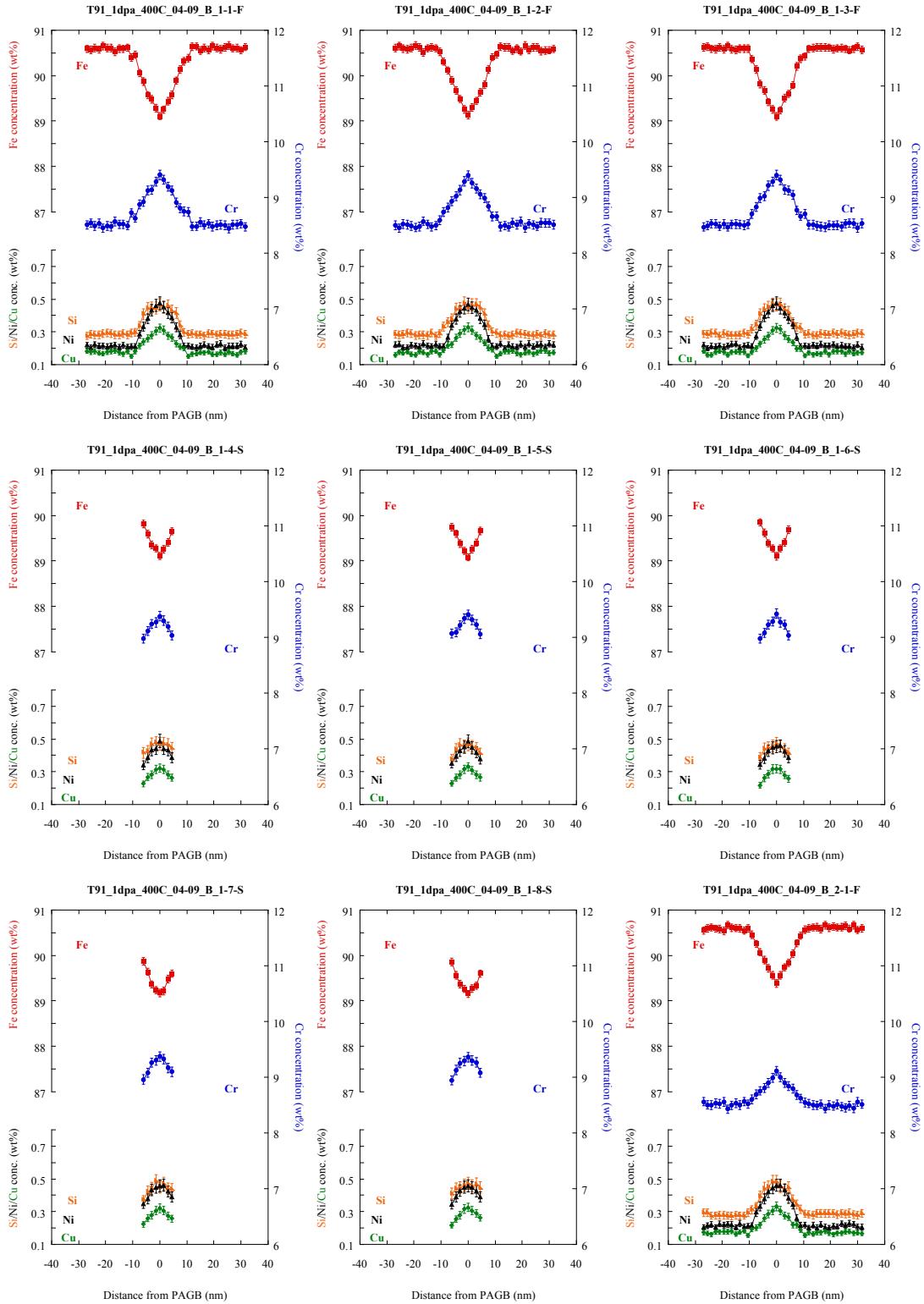
## HCM12A\_UI

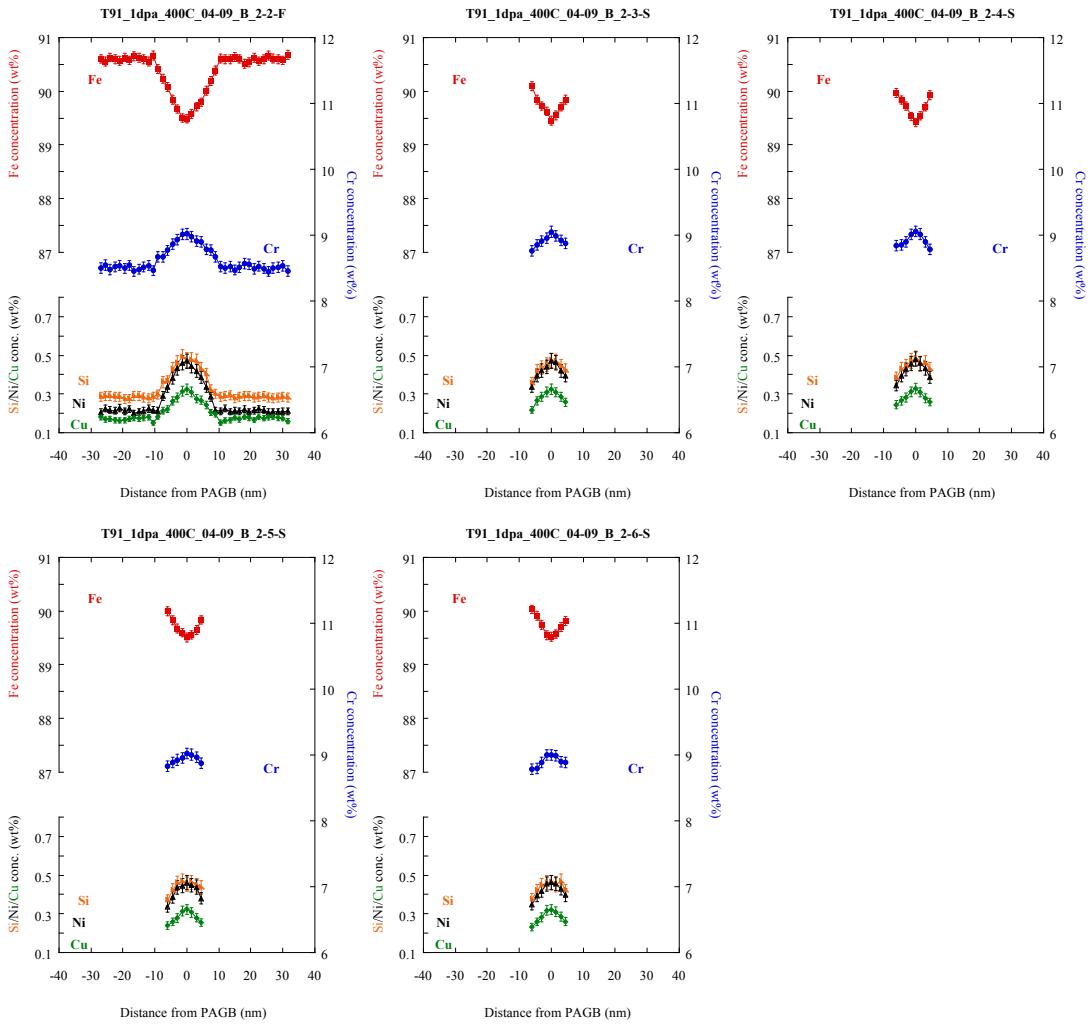


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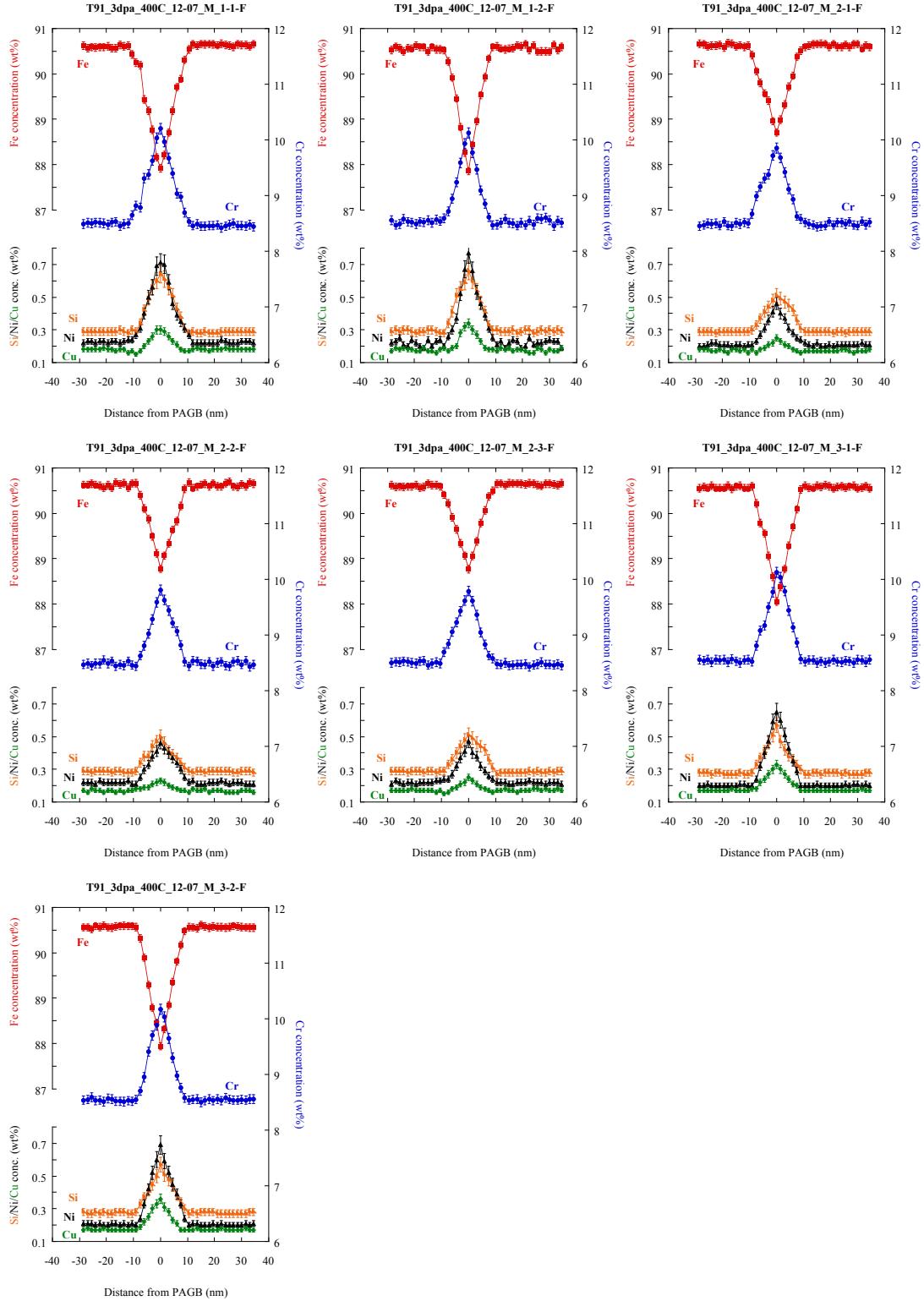


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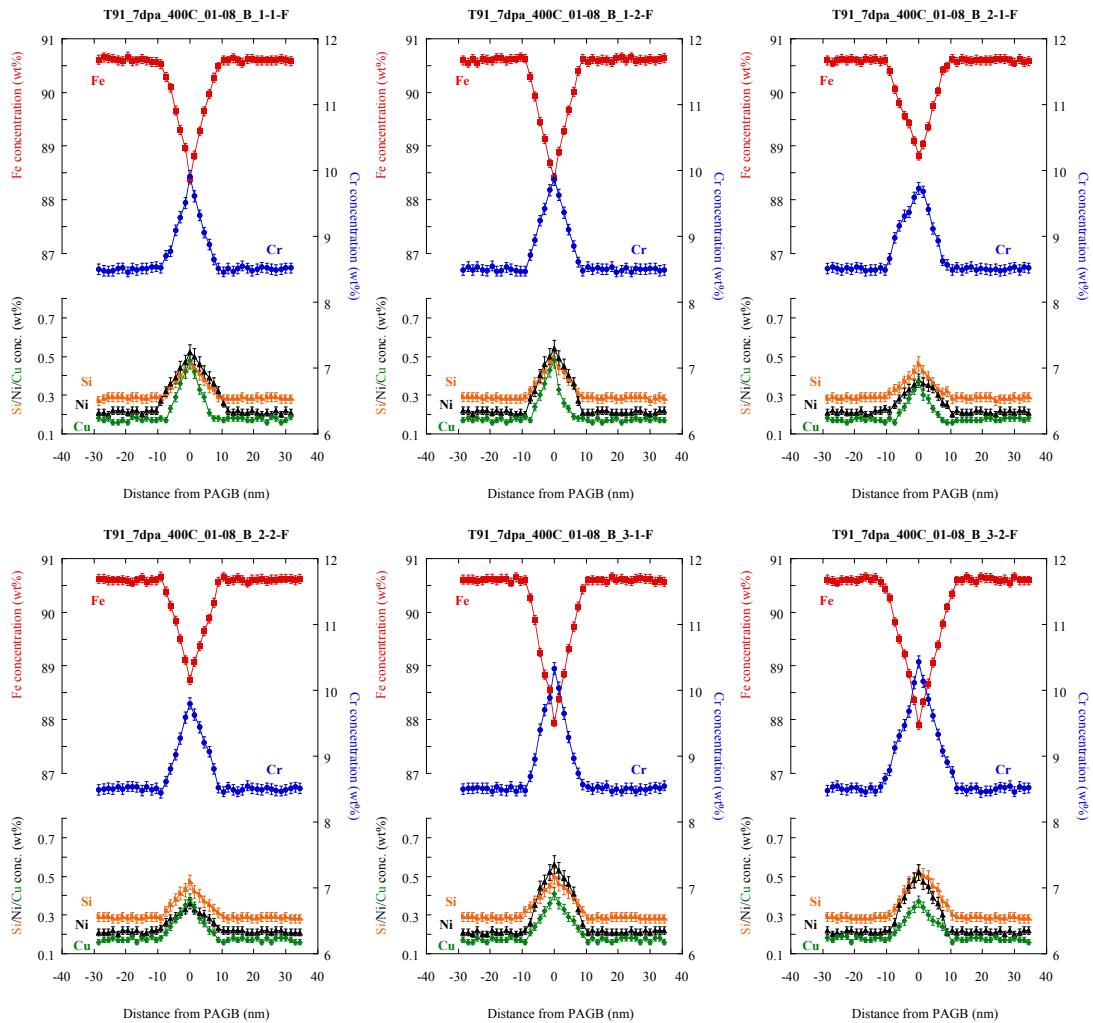




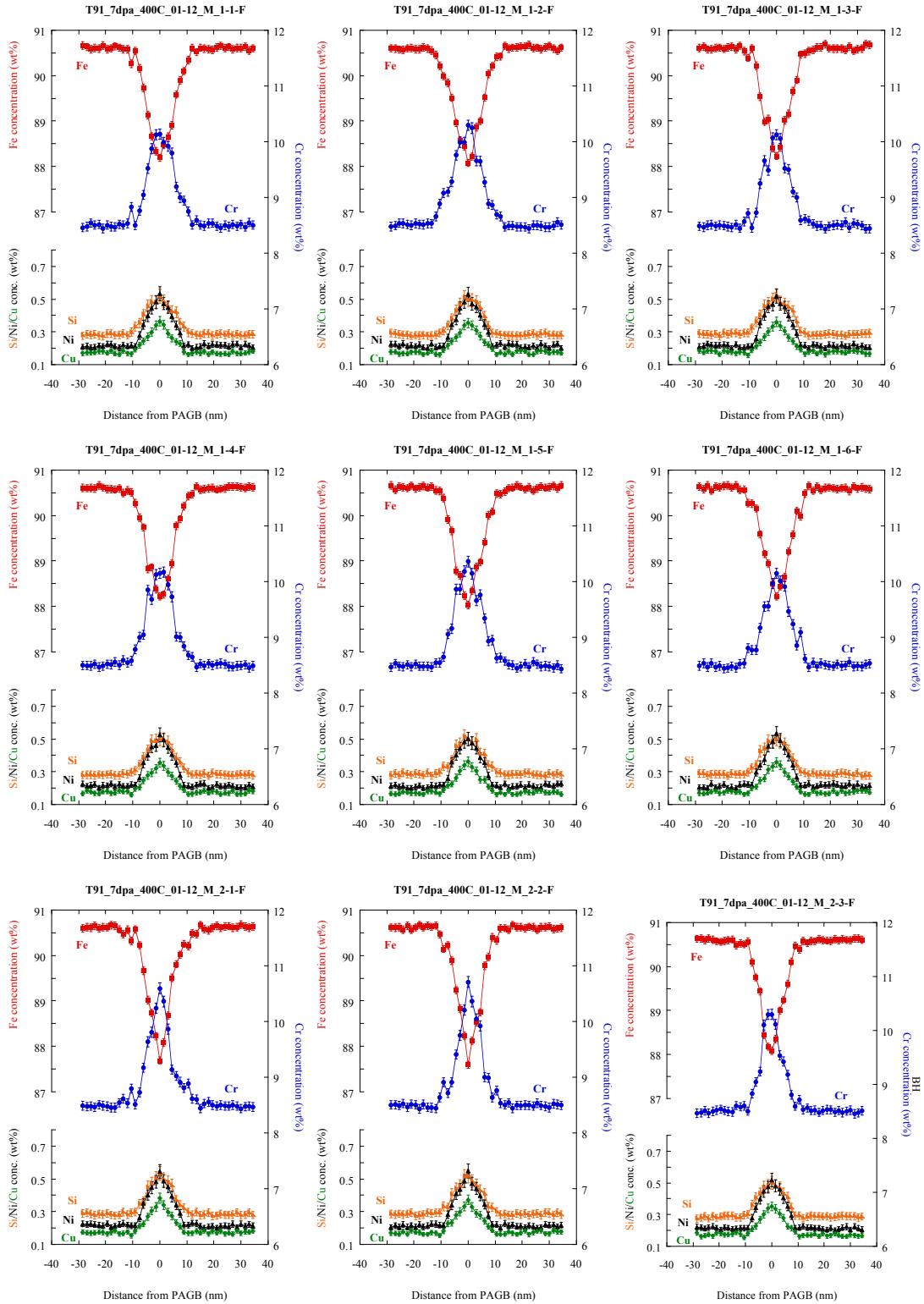
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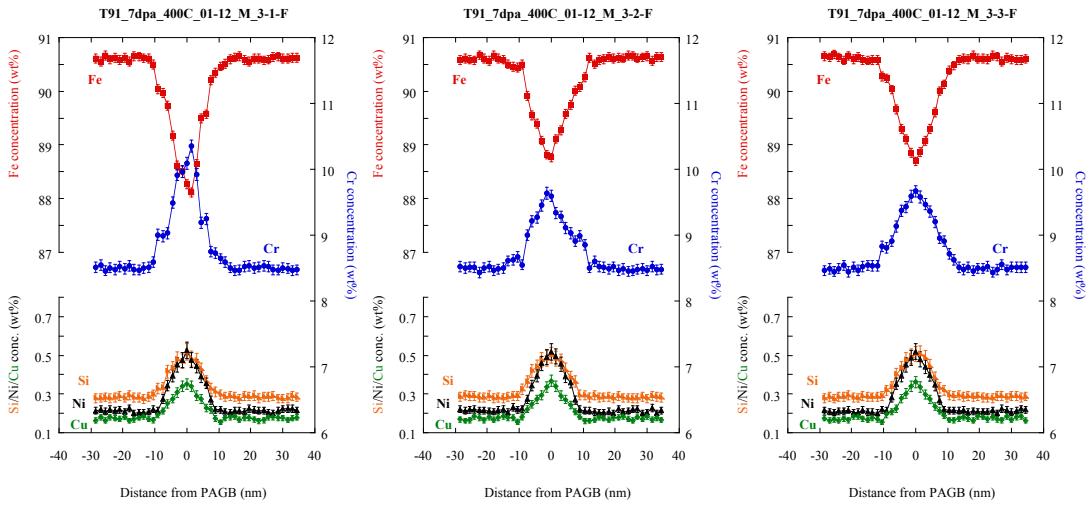


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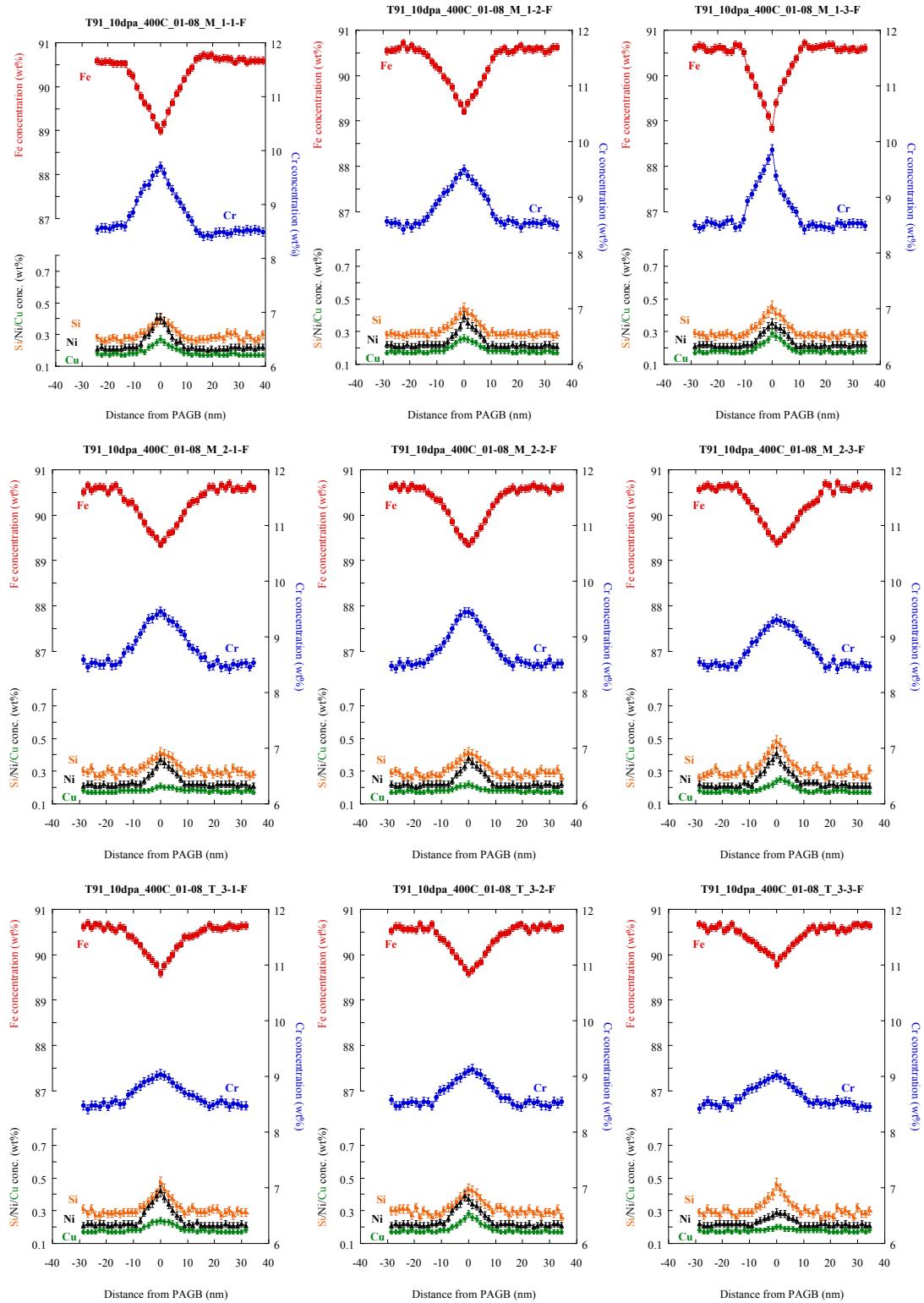


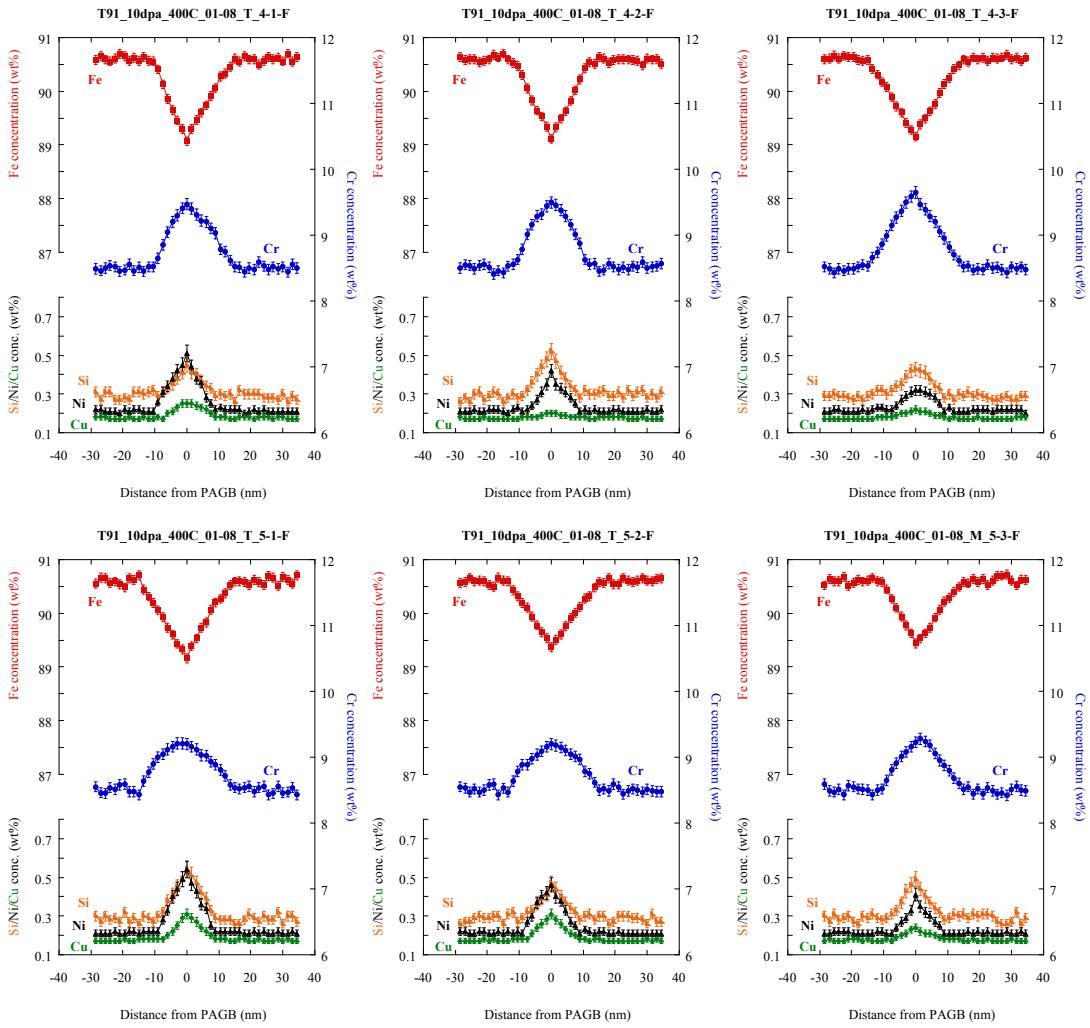
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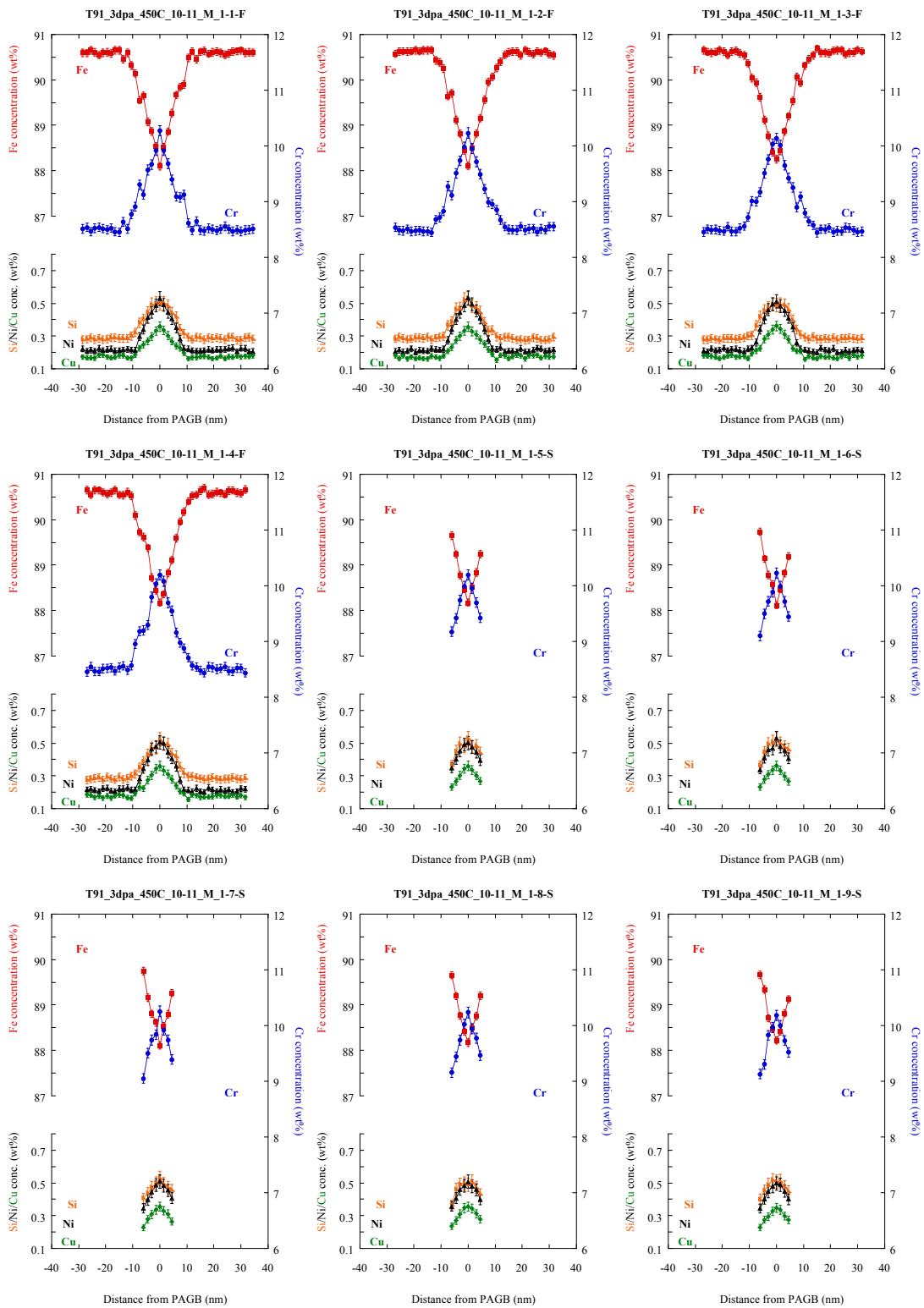


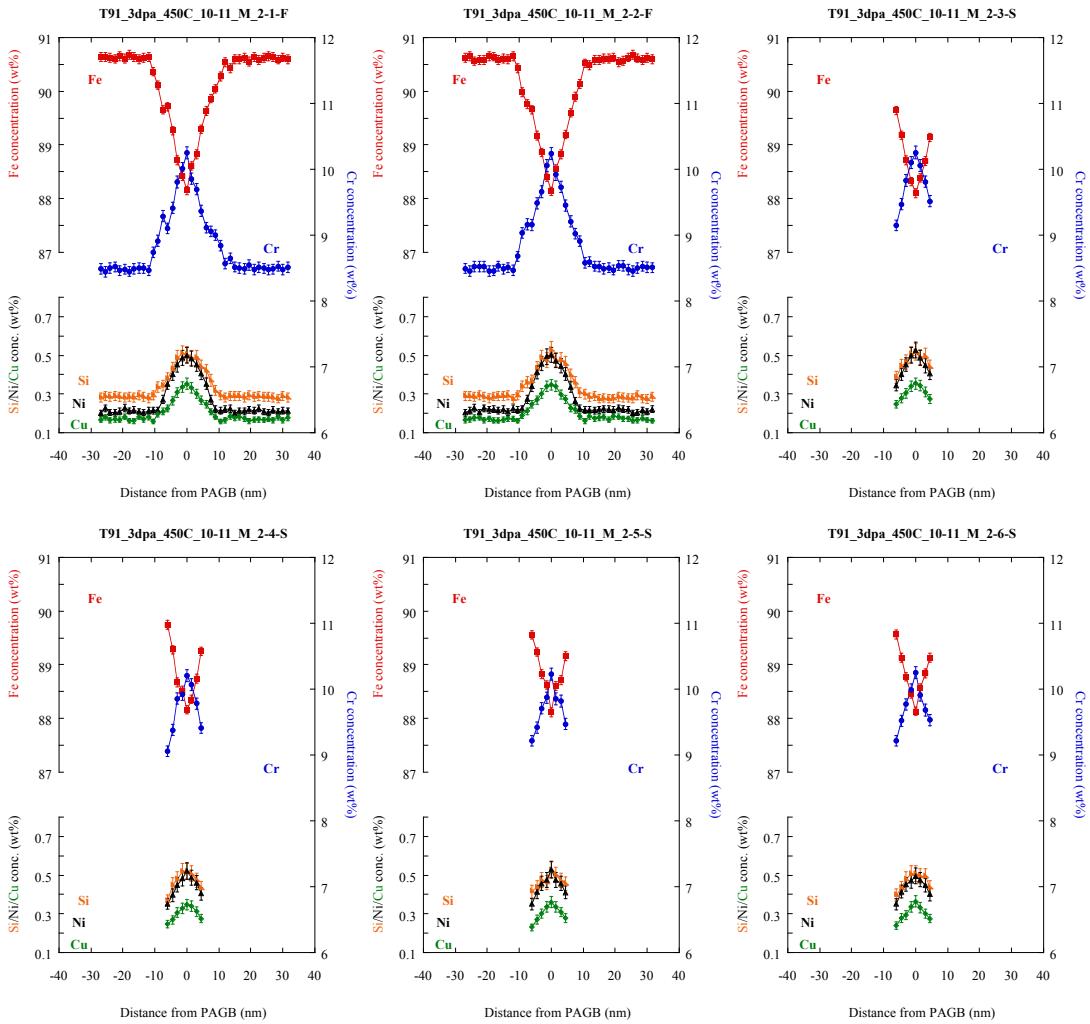
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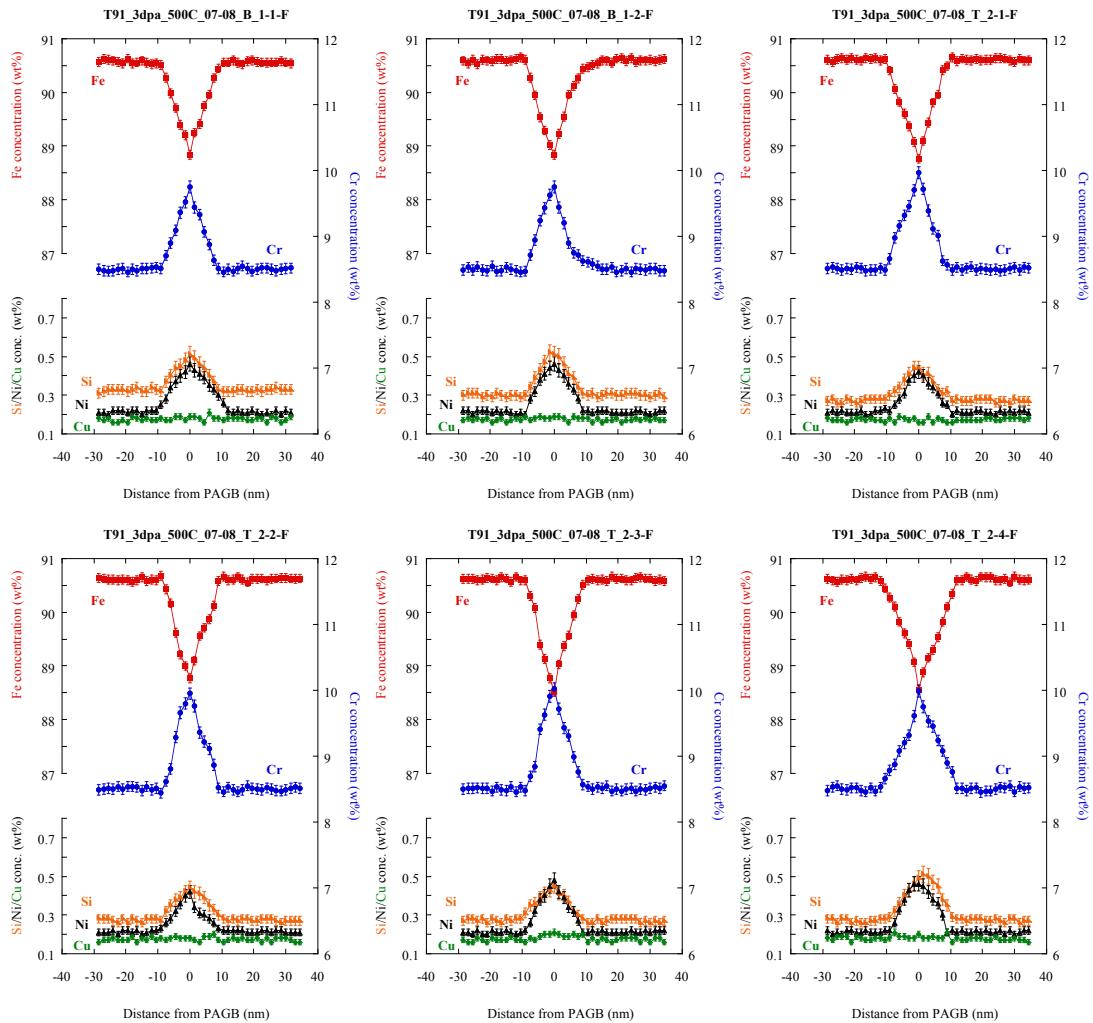


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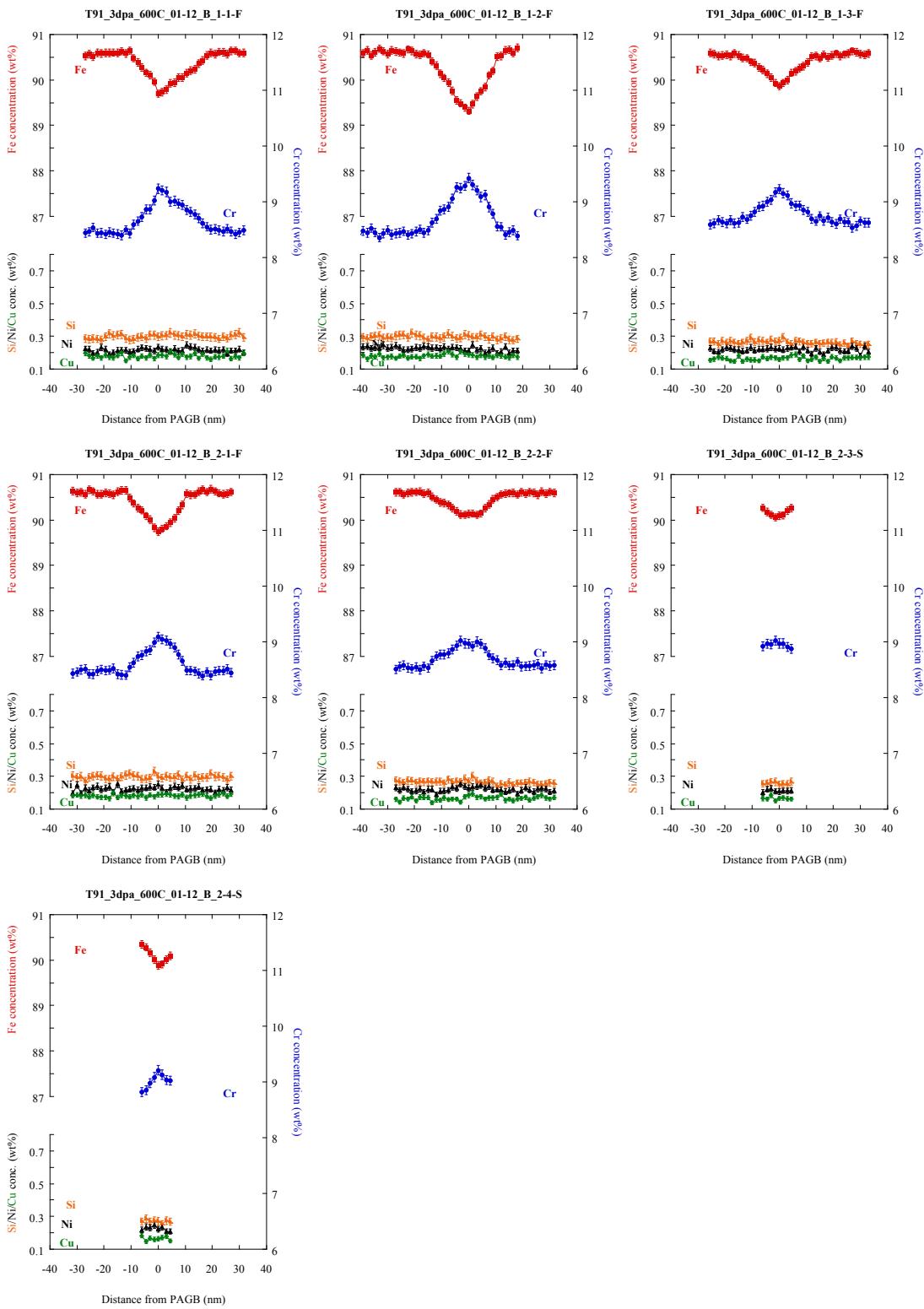




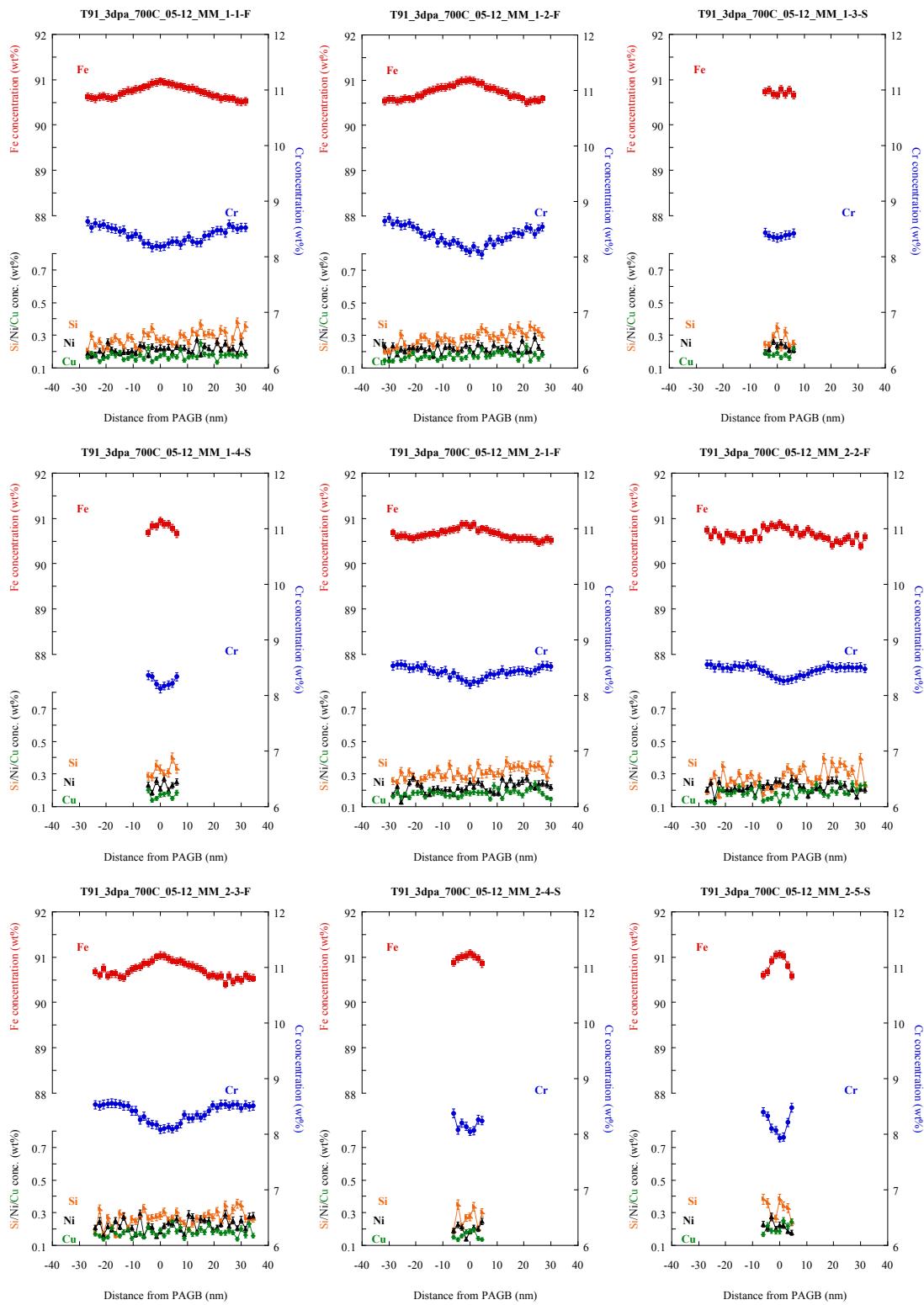
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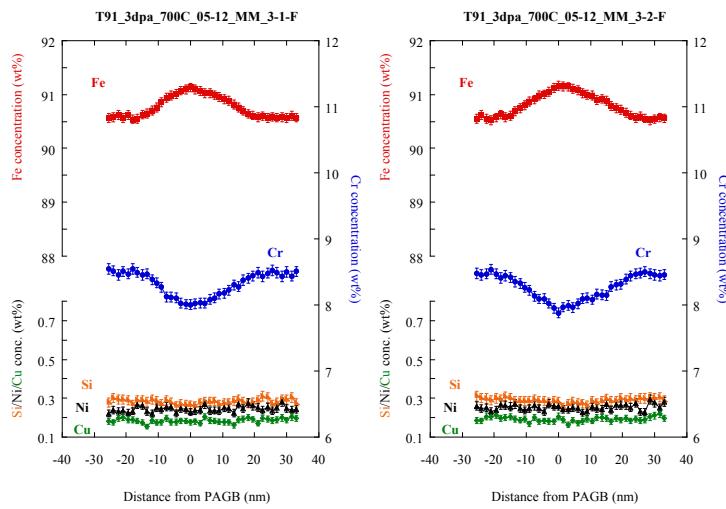


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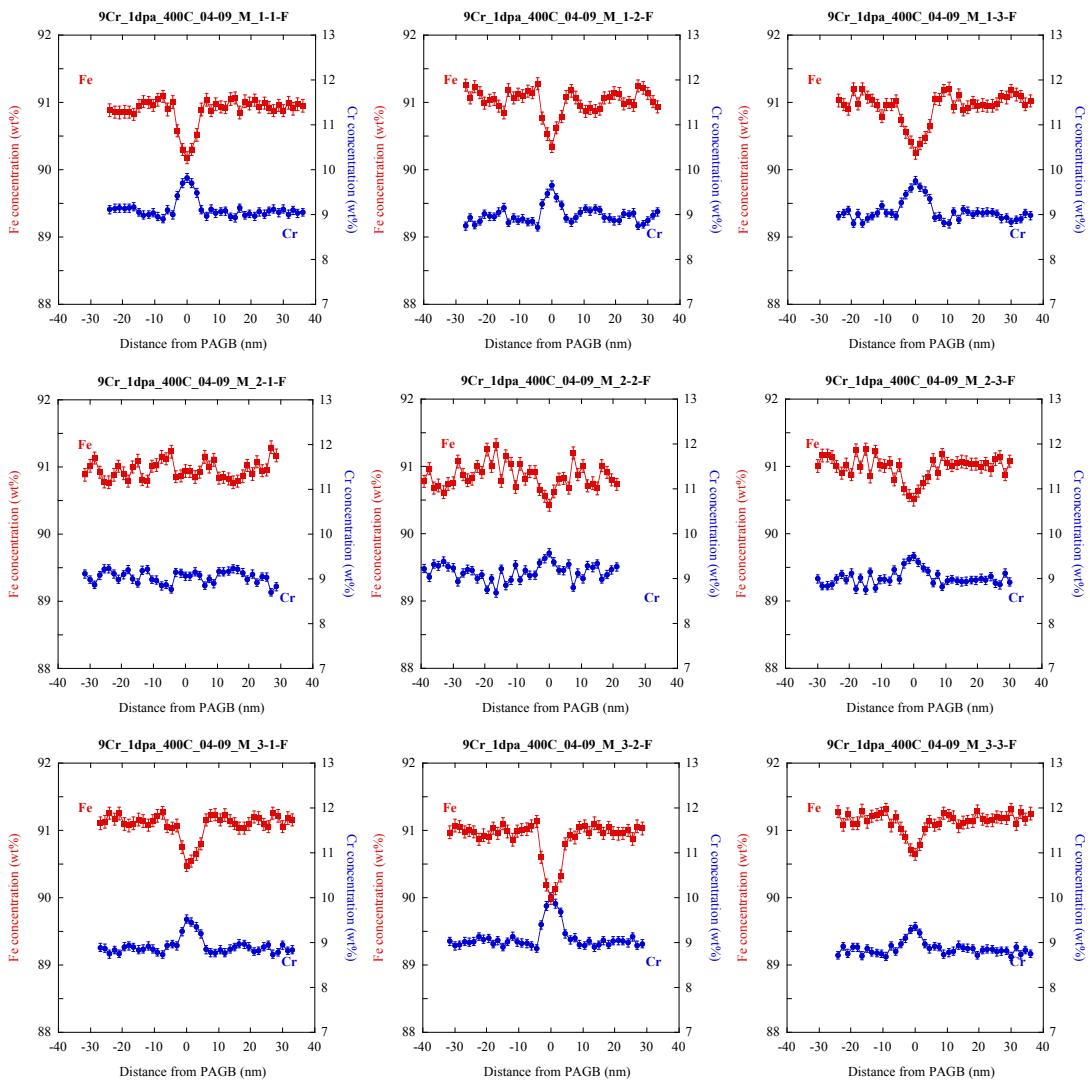


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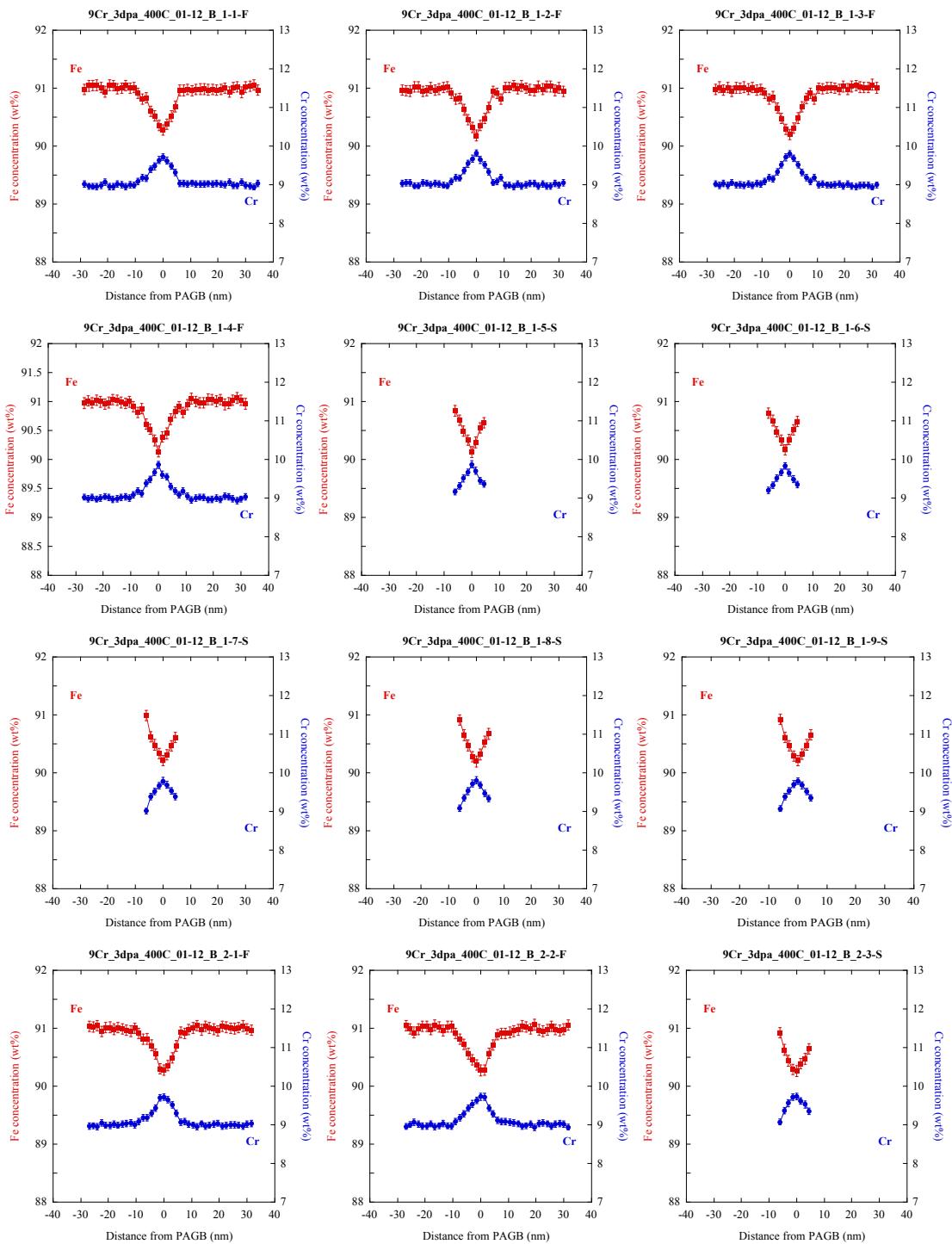


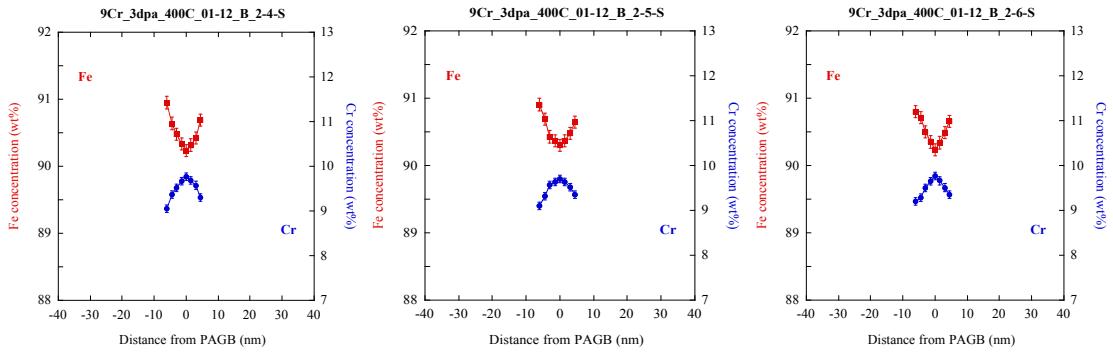


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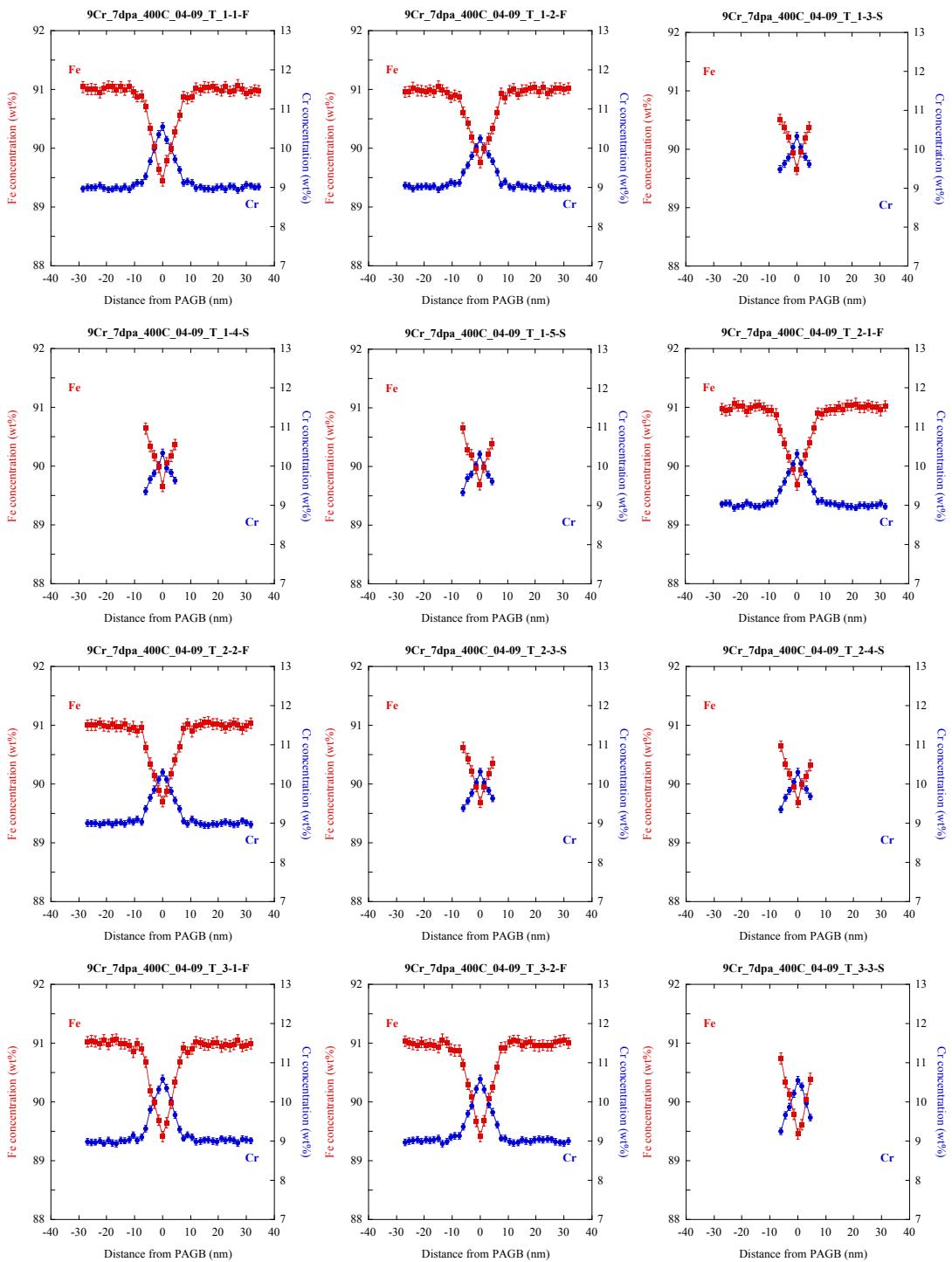


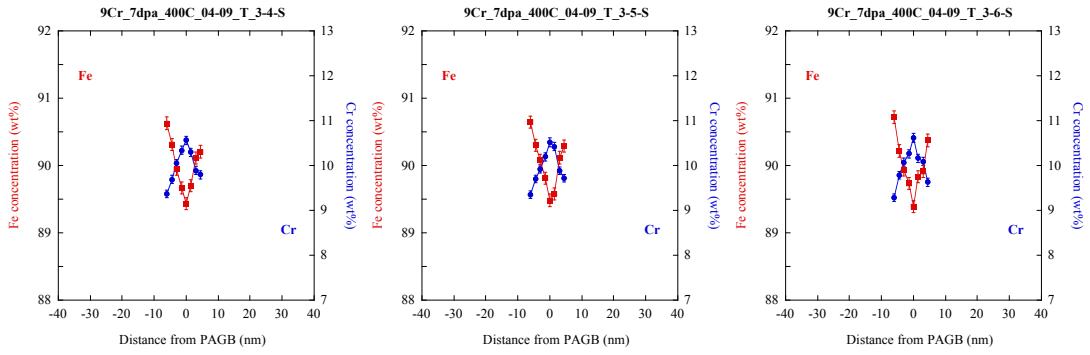
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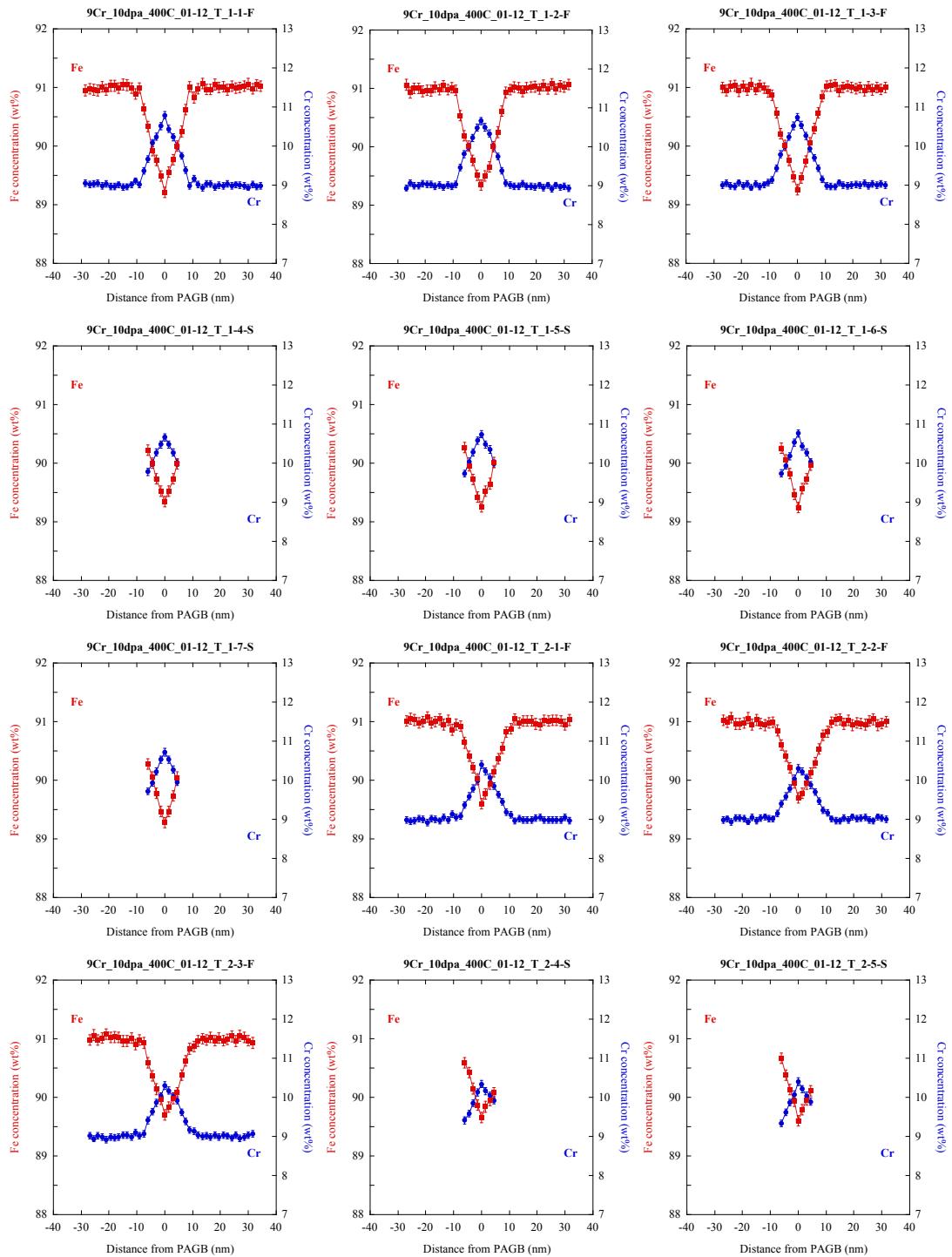


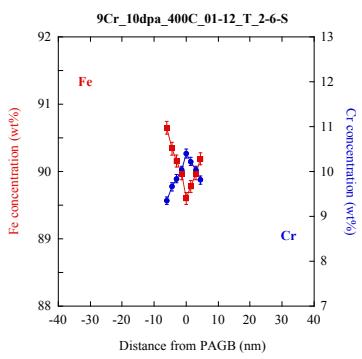
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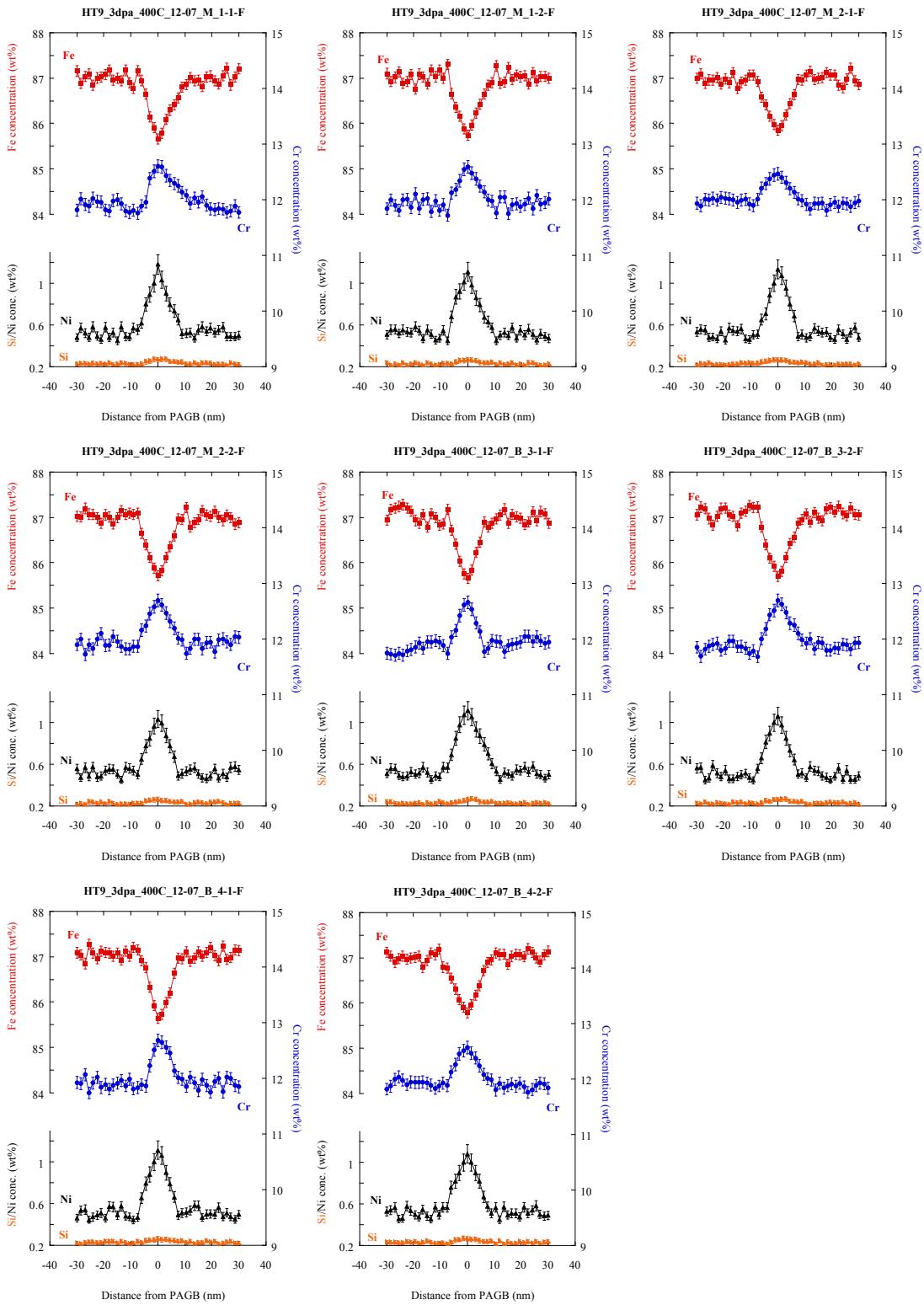


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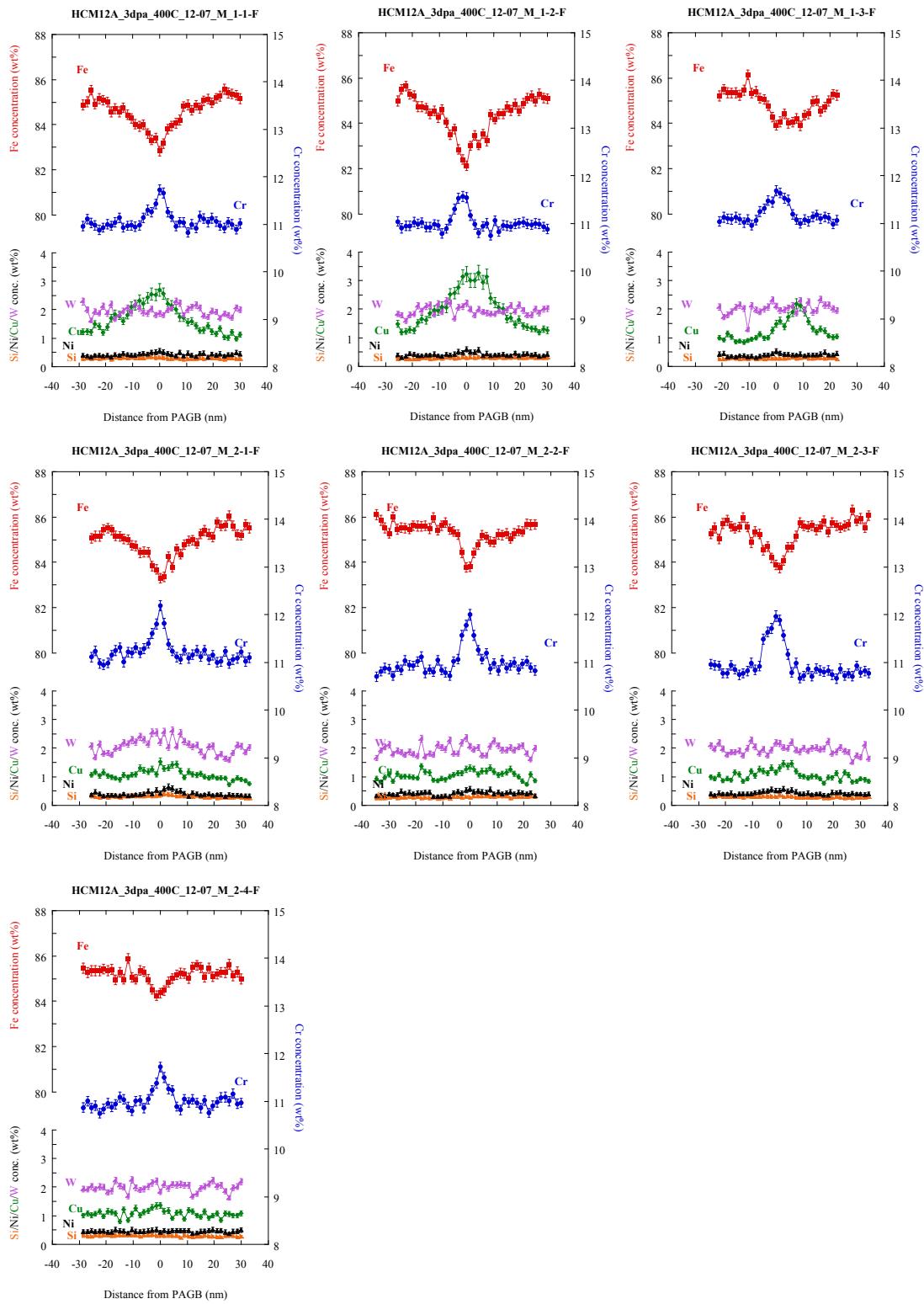




## HT9\_3dpa\_400C\_12-07



## HCM12A\_3dpa\_400C\_12-07



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