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Future prospects for intra-cluster medium enrichment studies

7.1 Current limitations of abundance measurements

Throughout this thesis, we have seen repeatedly that systematic uncertainties dominate over statistical uncertainties for large samples of deep cluster observations. It would be difficult (if not impossible) to make an exhaustive list of all the limitations that could potentially affect the average X/Fe abundance ratios measured in the ICM by the XMM-Newton instruments. In this thesis (and based on additional work on RGS measurements of the O/Fe ratio by [de Plaa et al.] (2017)) we have discussed and quantified:

- the intrinsic scatter of the measurements\(^1\) (up to \(\sim 25\%\));
- uncertainties in the spectral models and plasma codes (mostly below \(\sim 20\%\), up to \(\sim 40\% - 50\%\) for Mg/Fe and Ni/Fe at a few specific plasma temperatures);
- uncertainties in the thermal structure of the ICM (up to \(\sim 20\%\));
- uncertainties in the Galactic absorption, potentially affecting the O and N abundance measurements, when available (up to \(\sim 40\%\) in a few specific cases);
- the difference in the extracted regions between different instruments, e.g. RGS vs. EPIC, or within the same instrument, e.g. EPIC 0.05\(r_{500}\)

\(^1\)Although the intrinsic scatter is partly natural and should not be considered as a systematic uncertainty, it clearly affects the total dispersion of our measurements and deserves to be well understood.
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vs. EPIC 0.2$r_{500}$ (up to $\sim$10%);

- uncertainties related to the cross-calibration between the instruments (up to $\sim$20%, depending on the energy band considered);

- uncertainties in the background and foreground modelling (difficult to quantify, as it depends on the data quality, the plasma temperature, the studied region, and the method used to deal with the background).

Apart from these limitations on the abundance ratios, we can also list additional systematic uncertainties (usually difficult to quantify) that may affect the abundance measurements in general:

- projection effects;

- possible unaccounted radiative effects (charge exchange, resonant scattering, etc.);

- uncertainties related to possible spatially unresolved substructures with possibly different enrichment levels.

Some items can be identified as systematic effects from spectral fitting (e.g. atomic uncertainties, uncertainties in the Galactic absorption), while some others are clearly due to the limitations of the current instrumentation (e.g. cross-calibration uncertainties, non-X-ray background). In some cases, however, the distinction is less easy to do. For instance, the uncertainties in the ICM thermal structure are related to both the choice of the thermal model in the fits (single-temperature, $g_{\text{dem}}$, etc.) and to the limited spectral resolution of the instruments, which prevents to favour any particular thermal model.

One more complication is that some uncertainties might depend on others. For instance, if the studied region of the ICM contains unresolved substructures (for example small clumps of cold, enriched gas), this will have a simultaneous impact on (i) the derived average abundances directly and (ii) the derived average temperature and/or the assumptions made on the temperature structure. In turn, this incorrectly modelled temperature structure may play a role in bringing further uncertainties on the (already biased) average abundances.

What needs to be done to further improve our measurements? The answer to this question is not trivial, as it depends on which uncertainties one
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wants to reduce. While deeper individual exposures with current missions may help to better understand some limitations (Sect. 7.2), it is clear that substantial efforts should be pursued on other aspects. In particular, the two most crucial improvements that are needed are

1. improvements on the spectral codes and atomic calculations (Sect. 7.3);
2. more advanced X-ray instruments, including better spectral resolution, spatial resolution, and effective area (Sect. 7.4 and 7.5).

Finally, further comprehensive studies on Galactic absorption effects, on the X-ray background and foreground, and on how to interpret the projected spectra (e.g. using mock datasets from 3-D chemodynamical simulations) would also help to better understand and correct some of the systematic biases mentioned above.

7.2 The future of XMM-Newton in intra-cluster enrichment studies

7.2.1 Nearby clusters and supernova models

Since, for large nearby samples like the CHEERS sample, systematic uncertainties of the abundance measurements dominate over the statistical ones, collecting more photons will not help to improve significantly the results that were obtained in this analysis. Therefore, one of the most important take-home messages of this thesis is that we have probably reached the limits of what can be possibly achieved with XMM-Newton.

This conclusion, however, should be somewhat nuanced. First, as discussed by de Plaa et al. (2017), the high quality of the data may be used to reveal unexpected systematic biases. In turn, this may lead to a better understanding of some systematic uncertainties, and contribute to substantially improve the global accuracy of the results. Second, deep observations of each object of the sample are very useful to constrain and eventually better understand the intrinsic scatter. Outliers can be then isolated and studied in more detail. Finally, increasing the exposure of each source of the CHEERS sample would allow to build detailed 2-D metal maps and study the possible azimuthal asymmetries in a more comprehensive way.

In addition to the systematic uncertainties discussed above, the interpretation of our measured abundances is limited by the accuracy of the
current SN models. Indeed, when one wants to constrain SN models from the ICM abundance ratios, additional uncertainties affecting the yield predictions should be also considered. They may be due to the input physics, the initial conditions and assumptions, or the computational methods that were used. For example, similar SNcc yield models proposed in the literature by different groups do not perfectly agree (see e.g. De Grandi & Molendi 2009; Nomoto et al. 2013). Such discrepancies are also found in SNIa yield models, for example when comparing one- and multi-dimensional approaches, or when using updated electron capture rates (Maeda et al. 2010, see also Chapter 4). In that respect, it will be crucial to improve the convergence between the SN yield predictions obtained by the different groups over the next few years.

Regardless of the future convergence between the nucleosynthesis yield models for SNIa explosions, another possible improvement that may be achieved by the SNIa theoretical community is on the yields predicted by the different SNIa progenitor channels. As explained in Chapter 4, the main unsolved question regarding SNIa is whether they occur in a single-degenerate (SD) or double-degenerate (DD) system. Since we have shown that ICM observations can easily favour and/or rule out some explosion mechanisms, a clear differentiation of the yields predicted by SD and DD scenarios would also allow us to bring substantial clues on the dominant SNIa progenitor channel. If the white dwarf (WD) density is high, electron captures are quite efficient and produce large amounts of neutronised species, such as $^{58}$Ni and $^{55}$Co, further decaying into $^{55}$Mn. If we assume the SD channel to result from a slow accretion by the WD (thus approaching the Chandrasekhar mass, $M_{\text{Ch}}$) and the DD channel to result from the direct merger between two WDs (whose masses remain well below $M_{\text{Ch}}$), the SD scenario should produce significantly more Mn and Ni than the DD scenario (e.g. Seitenzahl et al. 2013a; Yamaguchi et al. 2015). Unfortunately, the total uncertainties of these two elements in the ICM are still large. Moreover, Mn is also affected by the initial metallicity of the WD progenitor, while Ni is also sensitive to the SNIa explosion mechanism itself. Therefore, the accurate predicted yields of more elements are also needed.

In Chapter 4, we have shown that our measured ICM abundance pattern does not match the yield predictions of a violent collision between two WDs of similar masses ($\sim 0.9 \, M_{\odot}$ each, Pakmor et al. 2010). This does not necessarily mean that all violent WD-WD collisions are to be discarded as SNIa progenitors, because at this stage the dependency of the relative
yields on the different parameters of the merger (e.g. the WD-WD mass ratio) is still unclear. Moreover, the DD scenario could even be possible in a sub-$M_{\text{Ch}}$ case, where the most massive WD slowly accretes the disrupted material of the less massive WD (e.g. Piersanti et al. [2003]). In that context, if efforts are pursued by the SNIa community to predict the differences between the yields of all the SD and DD scenarios, our ICM abundances will be a valuable legacy that may help to solve the SNIa progenitor problem.

7.2.2 High redshift clusters

Another question that arises is whether XMM-Newton can be useful for studying the enrichment at higher redshifts. Historically, after a first ASCA study showing no evidence of evolution in the ICM metallicity up to $z \sim 0.4$ (Mushotzky & Loewenstein [1997]), XMM-Newton and Chandra allowed to investigate clusters up to $z \sim 1.3$, and more recent work suggests a slight decrease of Fe abundance with redshift (Balestra et al. [2007]; Maughan et al. [2008]; Anderson et al. [2009]; Baldi et al. [2012]). These results, however, are not always confirmed (e.g. Tozzi et al. [2003]). In fact, if the core-excised regions only are considered, a flat trend even beyond $z \sim 1$ would not be surprising, as the early enrichment in the outskirts is expected to have occurred already before that epoch (Chapters [1] and [3]). That being said, a clear redshift-metallicity trend is difficult to confirm, because of possible intrinsic dispersion in the measurements. Moreover, the statistical errors on the metallicities of higher-$z$ clusters are often large ($\gtrsim 30\%$).

Recently, de Plaa & Mernier (2017) estimated that, to clearly separate a flat from a decreasing trend with 90% of probability, observations of about 150 clusters within $0.3 < z < 1.0$ would be needed, with a total net exposure time of $\sim 13.7$ Ms. Although technically feasible, the chances to obtain such a large total exposure in the upcoming XMM-Newton observation rounds are low.

7.3 Future work on atomic data and spectral modelling

In Chapter 5, we showed that updates in atomic codes may provide significant effects on the abundance determination. This clearly illustrates the importance of such improvements if one wants to further constrain the abundances and better interpret the ICM enrichment.

Despite the remarkable improvements of SPEXACT v3 compared to its
7.4 X-ray micro-calorimeters

previous version, current models hardly reproduce specific spectral features in cool \((kT \lesssim 1\ \text{keV})\) plasmas, in particular in the Fe-L complex (Chapter 5). This clearly shows that further efforts toward more complete spectral modelling is desirable. These efforts can be led on different aspects: better calculations of the ionisation processes and the overall ionisation balance (e.g. \cite{Urdampilleta2017}), better parametrisation of the radiative recombination rate coefficients (e.g. \cite{Mao2016}), implementing more spectral transitions into plasma codes (not only for H-like and He-like ions, but also for more complex electronic sequences), and/or a continuous and self-consistent update of the atomic data.

The optimal way to test our current knowledge of the radiation processes in CIE plasmas is to compare the current models with the most detailed data available. While laboratory experiments may be useful in some specific cases (e.g. \cite{Beiersdorfer2004, Shah2016}), it is not possible to recreate the exact ICM conditions in laboratories (for instance, forbidden transitions observed in astrophysical plasmas require very low densities that cannot be currently achieved on Earth). Instead, the very first spectra of the ICM made by the new generation of X-ray satellites (Sect. 7.5) will be extremely useful to confront with the up-to-date models from SPEXACT (cie or gdem) and AtomDB (apec).

Above all, it is essential to understand the origin of the current discrepancies between the different spectral codes. Parallel ongoing improvement of SPEXACT and AtomDB will certainly improve the convergence between the prediction made by these two codes, and will clearly help to reduce the atomic uncertainties of our abundance measurements.

7.4 X-ray micro-calorimeters

In addition to atomic data, the most constraining limitation of the current X-ray instruments (i.e. CCDs and grating spectrometers) in the abundance measurements is their spectral resolution. In fact, many of the systematic uncertainties listed in Sect. 7.1 will be better understood with a better resolution of the emission lines in X-ray cluster spectra. More generally, improved spectral resolution will bring our understanding of the spectroscopy in the ICM (and hot plasmas in general) to another level. This will, in turn, considerably enlarge our current knowledge of metal enrichment in the ICM. Currently, the next step toward a better spectral resolution is the use of X-ray micro-calorimeters in future missions.
A micro-calorimeter is essentially made of three components: a X-ray absorber, a thermistor, and a heat sink (Fig. 7.1 left). The absorber and the heat sink are connected by a thermal link. On paper, the principle is quite simple. When a X-ray photon hits the absorber, its incoming energy is converted into a small heat increase, which is measured by the thermistor. This heat increase causes a change in resistance of the thermistor before being dissipated by the heat sink. The current through the thermistor is measured continuously, and from the pulse signal detected in the current, the photon energy can be derived with high precision. One good example of micro-calorimeter is the transition-edge sensor (TES), which will be used in the X-IFU instrument of Athena (Sect. 7.5.3). The material used as thermistor in TES-like micro-calorimeters is actually superconducting at very low temperature, while it quickly reaches a threshold of constant electrical resistance ($R_{\text{TES}}$) at higher temperature. In between (i.e. in the transition edge between the two regimes), a small change in temperature will result in a strong change in $R_{\text{TES}}$ (Fig. 7.1 right). In that sense, the thermistor acts like an extremely sensitive thermometer, as its resistance can be used to efficiently measure small temperature changes caused by absorbed X-ray photons.

In the absorber, the incident photon energy ($E$) is simply proportional
to the heat variation ($\Delta T$):

$$\Delta T \propto \frac{E}{C}, \quad (7.1)$$

where $C$ is the heat capacity of the absorber. Since $\Delta T/T$ is typically of the order of 0.01%, the heat sink must keep the absorber as close as possible to the absolute zero in order to minimise the thermal noise. This implies the need for a complex unit efficiently cooling the detector. Moreover, the absorbing material should have its heat capacity as low as possible, and should be efficient in absorbing X-rays.

Compared to CCD (or proportional counter) detectors, the main advantage of micro-calorimeters resides in their remarkable energy resolution ($\Delta E$). For CCDs, $\Delta E$ depends on both the photon energy and the number of the subsequent collected electrons ($N$), as

$$\Delta E \propto E \sqrt{\frac{N}{N}}, \quad (7.2)$$

On the other hand, it can be shown that for micro-calorimeters,

$$\Delta E \propto \sqrt{\frac{kT^2 C}{\alpha}}, \quad (7.3)$$

where $\alpha$ is the sensitivity of the thermistor. In other words, $\Delta E$ does not depend on $E$ and can potentially reach very low values (a few eV at most) if the detector is kept at very low temperatures. One limitation to the energy resolution is when two photons hit the absorber within a short interval implying that their subsequent temperature jumps cannot be clearly separated. In most clusters, however, the count rate of the ICM emission is weak enough to limit such a pile-up effect.

One of the main challenges for the next X-ray detectors is to build an array of independent micro-calorimeter units, thereby recreating a full grid of pixels and allowing to perform spatially-resolved spectroscopy. So far (i.e. in the SXS instrument, Sect. 7.5.1 and 7.5.2), each pixel is wired independently to the read-out electronics, which limits the number of pixels on the detector (to 36 in the case of SXS). In future instruments (e.g. X-IFU, Sect. 7.5.3), multiple pixels will be connected to one read-out chain, although they can still be read-out independently using a multiplexing technique. This will allow to create more pixels per detector (~3500 approximately), and to reach a good spatial resolution while keeping an exquisite spectral resolution.
7.5 The upcoming generation of X-ray missions

As seen in Sect. 7.4, X-ray micro-calorimeters have a substantially improved spectral resolution compared to the instruments used in X-ray missions so far. This would be essential to further constrain abundances in cluster X-ray spectra. Fortunately, the upcoming generation of X-ray missions are (or will be) equipped with micro-calorimeters. In this section we briefly discuss the potential improvements that these missions may bring to the ICM enrichment.

7.5.1 Hitomi

On 17 February 2016, the Japanese satellite Hitomi (previously ASTRO-H, Fig. 7.2; Takahashi et al. 2014) was successfully launched. In addition to the two gamma-ray detectors and the two hard X-ray telescopes, the mission included two soft X-ray telescopes which focused light onto a soft X-ray imager (SXI) and a micro-calorimeter instrument — namely the soft X-ray spectrometer (SXS). The latter had a field of view of 3x3 arcmin and a very high spectral resolution of $\sim$5 eV, allowing to do high-resolution spectroscopy in the 0.4–12 keV band at an unprecedented level. The first observation made by SXS (initially for calibration purposes) was the core region of the Perseus cluster in the 2–10 keV band. Unfortunately, about one month after the launch, the satellite experienced a loss of communication. It was later discovered that a chain of anomalies in the attitude control system caused an uncontrollable spinning of the satellite. Due to the subsequent accumulation of excessive momentum, several parts of the spacecraft eventually broke away. Despite all the efforts from JAXA to recover it, the mission was officially aborted on 28th April 2016.

Although this early end of Hitomi was very bad news for the whole X-ray astrophysics community, the observation of Perseus has been a great success in terms of technical capabilities (e.g. Hitomi Collaboration et al. 2016). Above all, the mission revealed the exquisite spectral resolution that micro-calorimeters can realistically achieve (Fig. 7.3), thereby opening a new window on the future of ICM enrichment studies. An overview of the prospects of Hitomi in cluster physics is given by Kitayama et al. (2014).
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**Figure 7.2:** Artist impression of the *Hitomi* satellite (Credit: JAXA).

**Figure 7.3:** *Hitomi* SXS spectrum of the core of the Perseus cluster (*Hitomi Collaboration et al.* 2016). Overlaid in red is a typical CCD spectrum (*Suzaku* XIS) extracted from the same region.
7.5.2 XARM

The success of the SXS instrument onboard *Hitomi* to resolve metal lines in the spectrum of Perseus has been a strong motivation to recover the mission. On 14 July 2016, JAXA announced that a successor of *Hitomi* is actually planned for the year 2021. Named the *X-ray Astronomy Recovery Mission (XARM)*, this satellite would be essentially centred on the SXS instrument.

If this mission is indeed confirmed, its SXS instrument will be highly valuable to future ICM enrichment studies. In Fig. 7.4, we simulate a SXS observation of 100 ks of cleaned exposure of the core region of Abell 4059 (see also Chapter 2). Here again, the simulated data illustrate the unprecedented spectral resolution we can achieve with a micro-calorimeter instrument.

One interesting direct application of the SXS capabilities is the improved measurement of the Ni/Fe ratio. As seen in Chapters 1, 4, and 5, the Ni/Fe ratio provides valuable constraints on the dominant SNIa explosion channel. Unfortunately, when measured with the EPIC instruments, this ratio suffers from large cross-calibration and background uncertainties (Chapter 3), and is very sensitive to the used spectral codes and atomic databases (Chapter 5). Moreover, at CCD spectral resolution, Ni-K lines are blended with Fe XXV (He-like) lines, thereby limiting the robustness of the Ni abundance measurement. In addition to be weakly affected by the instrumental background even at high energies, the SXS instrument is able to fully disentangle all the Ni and Fe lines, and will thus dramatically improve our measurement of the Ni/Fe ratio. Based on the simulation presented in Fig. 7.4, and assuming ongoing efforts are pursued toward an improvement of the plasma atomic codes, we estimate that the statistical errors on Ni/Fe should not be larger than \( \sim 8\% \). At that level of accuracy, it will be easy to determine which of the deflagration or the delayed-detonation explosion mechanism is the dominant one in SNIa.

Another significant progress that SXS will be able to achieve is a better quantification of the radial variation in the relative number of SNIa (SNcc) enriching galaxy clusters. As shown in Chapter 6, we have provided interesting hints that SNIa and SNcc enrich the ICM at the same level in the centre and in the outer parts (\( \sim 0.5r_{500} \)). This could be further confirmed

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\[2\] The main reason of the low background level of the SXS instrument is related to the choice of the low-Earth orbit of the *Hitomi/XARM* missions. This choice, however, also has drawbacks, like a shorter lifetime of the mission.
by pointing SXS successively toward the centre and an offset region of a cool-core cluster like Abell 4059. Since the instrumental background level of SXS is limited even at low surface brightness, it will be possible to measure the O/Fe and/or the Mg/Fe ratios with an excellent accuracy. Because O and Mg are produced in SNcc while Fe originates predominantly from SNIa, these two ratios are good indicators of the enriching SNcc-over-SNIa fraction in the studied regions of the ICM.

A third (and very interesting) contribution of SXS to the field resides in the substantial improvement of the measurement of the O, Ne, and Mg abundances. As discussed in Chapter 4, an accurate determination of the Ne/Mg ratio can in principle help to constrain the shape of the initial mass function (IMF) of the SNcc progenitors. This would be particularly valuable, since the question of the universality of the IMF is still under debate.
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Finally, in addition to substantially improving the accuracy of the metal abundances discussed throughout this thesis, the SXS will also allow to detect the presence of rare elements (Na, Al, etc.) in the ICM for the first time. Measuring the abundance of these elements will be particularly useful to further constrain the initial metallicity of the SNcc progenitors (e.g. Nomoto et al. 2013).

7.5.3 Athena

Despite its very promising performances, the micro-calorimeter instrument onboard XARM is limited by its moderate spatial resolution (with a point spread function of \(\sim 1.2'\)) and effective area (\(\sim 250 \text{ cm}^2\) at 1 keV). These limitations prevent studies of high-redshift clusters. Nevertheless, in a further future, the European mission Athena (Fig. 7.5, expected launch in 2028) is expected to overcome this issue.

Athena will be essentially composed of two key instruments: a micro-calorimeter — the X-ray Integral Field Unit (X-IFU; Barret et al. 2013) — for high spectral resolution imaging, and a Wide Field Imager (WFI; Rau et al. 2013) for moderate spectral resolution imaging, covering a larger field of view. Compared to SXS, the main improvements of X-IFU will be its significantly better spatial resolution (with an expected point spread function of \(5''\)) and effective area (expected to be \(\sim 2 \text{ m}^2\) at 1 keV). This will allow to investigate metals with exquisite details not only in nearby clusters but also in more distant systems. For example, assuming 100 ks of cleaned ex-
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Figure 7.6: Simulated 250 ks spectrum of the core of a distant cluster ($kT = 3$ keV, $z = 1$) with the Athena X-IFU instrument. For comparison, similar simulated spectra are also shown for the XMM-Newton pn, Chandra ACIS-I, and Hitomi/XARM SXS instruments. For clarity, the data points have been rebinned to larger factors.
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Exposure, X-IFU will be able to detect O, Si, and Fe in clusters up to $z = 1$ and to measure their abundances with at least 10% of accuracy (Pointecouteau et al. 2013). We illustrate this by simulating 250 ks of cleaned exposure of a bright distant ($z = 1$) cluster ($kT = 3$ keV) with X-IFU, and by comparing its simulated spectrum with that of other instruments (Fig. 7.6). An overview of the prospects of Athena in cluster physics is given by Ettori et al. (2013).

7.6 Concluding remarks

Since the launch of Athena is expected for 2028, patience will be required before entering into this completely new era. Nevertheless, there is no doubt that this mission — together with XARM and the possible other X-ray missions that may be planned in a near future — will considerably expand our knowledge on the origin and distribution of metals in the ICM. While systematic uncertainties should always be borne in mind (as discussed above and throughout this thesis), we can reasonably hope that simultaneous and continuous improvements in ICM observations, ICM simulations, supernova models, instrument calibration, and atomic calculations will substantially reduce them.

Clearly, the future of chemical enrichment studies at the largest scales of the Universe looks promising and full of surprising upcoming discoveries.