

High-Temperature Volatilization of Cd, Te and CdTe, Revealed by the Skimmer Coupling

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Introduction

Cadmium telluride is an important semiconductor for thin-film solar cells, radiation detectors and optoelectronic devices. Its performance depends strongly on the Cd/Te ratio, phase purity and thermal stability. During deposition, annealing or recycling, preferential loss of Cd or Te can change the stoichiometry and affect material quality.

TGA-MS measurements are essential because TGA quantifies mass loss, while MS identifies the released species by their isotope-related mass traces. This allows the volatilization of elemental Cd and Te to be compared directly with the decomposition or evaporation behavior of CdTe. TGA-MS measurements using a skimmer system allow for a short gas transport path from the sample to the mass spectrometer and are particularly suited for substances prone to condensation, such as metals, salts, and high-boiling-point organic compounds. The combined information helps define safe and stable process windows for CdTe-based materials. The measurement conditions are detailed in Table 1.

Results and Discussion

The TGA-MS measurements show a clear correlation between the mass loss and the isotope-related ion-current traces for cadmium and tellurium. This is important because both Cd and Te have several naturally occurring isotopes. Therefore, the selected m/z traces do not represent single isolated signals, but characteristic isotope patterns that can be used to confirm the chemical identity of the released species.

Table 1 Measurement conditiosn

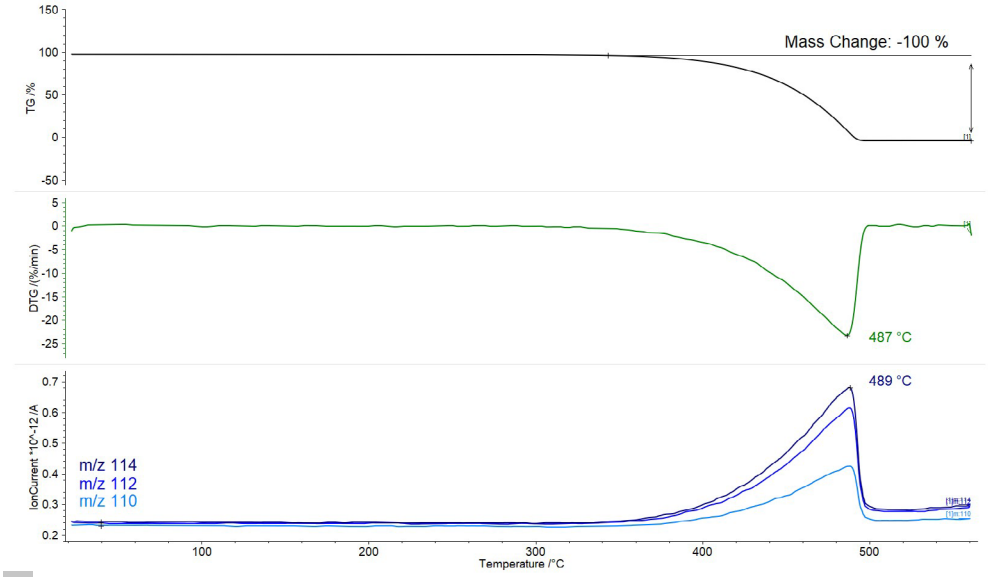
Sample	**Cd**	**Te**	**CdTe**
Sample mass	1.13 mg	1.00 mg	1.41 mg
Sample carrier	TGA Type S		
Furnace	Graphite Skimmer		
Curcible	Al_2O_3 crucibles, 85 µl, open		
Atmosphere	Purge gas: Helium, 50 ml/min Protective gas: Helium, 20 ml/min		
Temperature program	20 to 560°C	20 to 700°C	20 to 890°C
Heating zrate	10 K/min		

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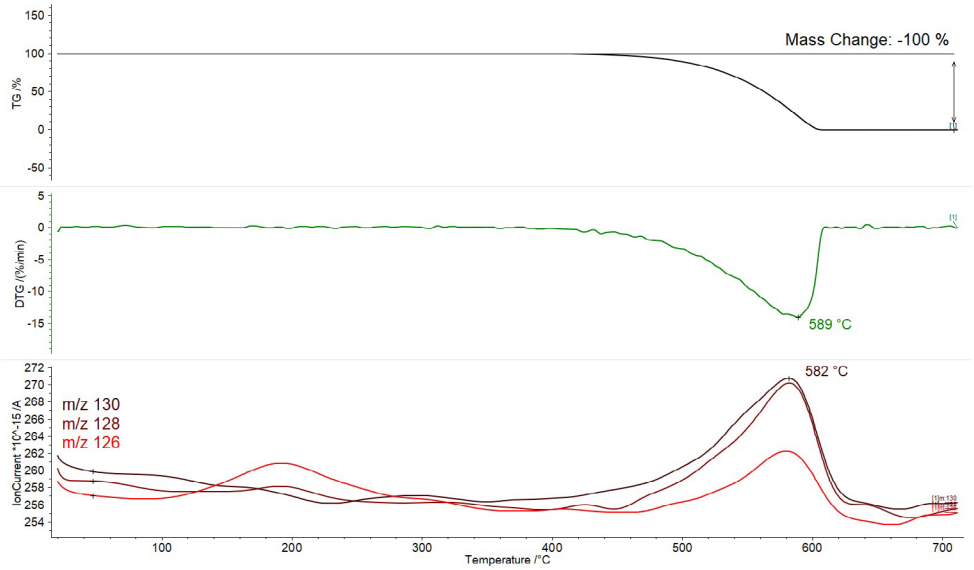
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For elemental cadmium, the TGA curve shows a complete mass loss, while the DTG signal exhibits its maximum at approximately 487°C (Figure 1). The Cd-related MS traces m/z 110, m/z 112 and m/z 114 reach their maxima at nearly the same temperature. These masses correspond to naturally occurring cadmium isotopes with abundances of approximately 12.5 % for ^{110}Cd, 24.1 % for ^{112}Cd and 28.7 % for ^{114}Cd. Accordingly, the expected intensity order is m/z 114 > m/z 112 > m/z 110, which is also reflected in the measured curves. The isotope pattern therefore confirms that the mass-loss step is caused by the release of cadmium-containing vapor species.

For elemental tellurium, the main mass-loss event occurs at higher temperatures (Figure 2). The Te-related MS traces m/z 126, m/z 128 and m/z 130 correspond to naturally occurring tellurium isotopes with abundances of approximately 18.8 % for ^{126}Te, 31.7 % for ^{128}Te and 34.1 % for ^{130}Te. The expected signal pattern is therefore m/z 130 ≈ m/z 128 > m/z 126. This relationship is consistent with the measured ion-current traces and confirms that the observed mass loss is associated with tellurium volatilization.



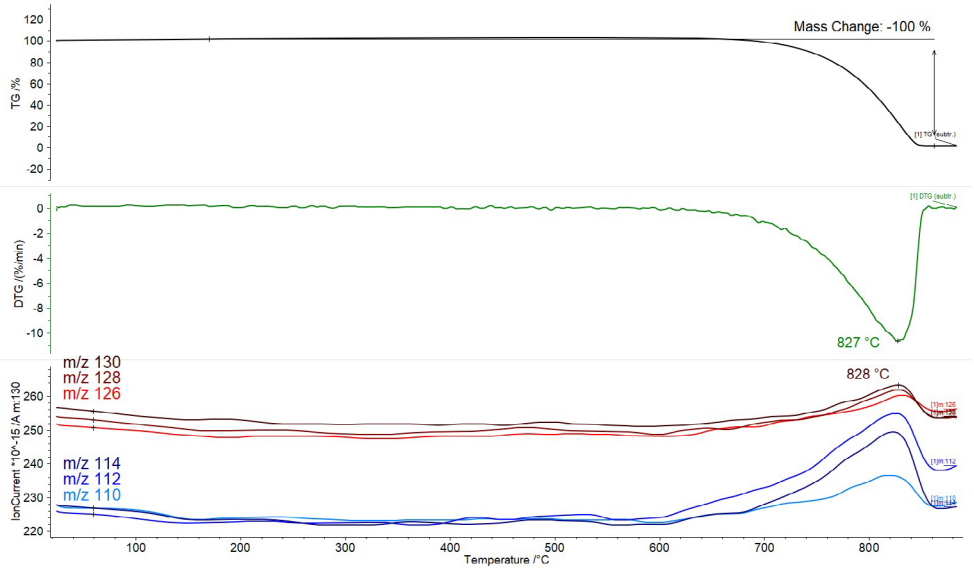
1 Mass change (TG, black), rate of mass change (DTG, green) and QMID curves for the mass numbers of Cd: 110 (light blue), 112 (blue) and 114 (dark blue) of the measured Cd sample.



2 Mass change (TG, black), rate of mass change (DTG, green) and QMID curves for the mass numbers of Te: 126 (light red), 128 (red) and 130 (dark red) of the measured Te sample.

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3 Mass change (TG, black), rate of mass change (DTG, green) and QMID curves for the mass numbers of Cd: 110 (light blue), 112 (blue) and 114 (dark blue) and Te: 126 (light red), 128 (red) and 130 (dark red) of the measured CdTe sample.

In the CdTe measurement (Figure 3), both isotope groups appear in the same high-temperature mass-loss region. The Cd-related traces m/z 110, m/z 112 and m/z 114 and the Te-related traces m/z 126, m/z 128 and m/z 130 increase simultaneously. Their relative intensities are consistent with the natural isotope distributions of Cd and Te, with ^{114}Cd and ^{130}Te, forming the strongest selected signals. This simultaneous detection shows that cadmium- and tellurium-containing species are released together during the high-temperature evaporation of CdTe.

Summary

The use of a NETZSCH TGA-Skimmer system is especially advantageous for these measurements because Cd and Te form heavy and condensable vapor species. The short, direct connection to the MS condensation is minimized, allowing the isotope-related MS peaks to be detected close to the corresponding DTG events. This is important for CdTe, where Cd- and Te-related signals occur in the same temperature range proving the evaporation of CdTe.

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